NERL Publication Report
Oct 16 – Oct 23, 2017

Published Articles & Reports

ORD-020010	Arango, C., J. Beaulieu, K. Fritz, B. Hill, C. Elonen, M. Pennino, P. Mayer, S. Kaushal, and D. Balz. Urban infrastructure influences dissolved organic matter quality and bacterial metabolism in an urban stream network. 2017. FRESHWATER BIOLOGY, 62(11): 1917-1928, https://doi.org/10.1111/fwb.13035	SED	Peer Reviewed	SSWR 4.2B

Impact / Purpose Statement
Cleared by NRMRL.
Published in the journal, Freshwater Biology.

Product Description / Abstract
Urban streams are degraded by a suite of factors, including burial beneath urban infrastructure, such as roads or parking lots, which eliminates light and reduces direct organic matter inputs to streams from riparian zones. These changes to stream metabolism and terrestrial carbon contribution will likely have consequences for organic matter metabolism by microbes and dissolved organic matter (DOM) use patterns in streams. Respiration by heterotrophic biofilms drives the nitrogen and phosphorus cycles, but we lack a clear understanding of how stream burial and seasonality affect microbial carbon use. We studied seasonal changes (autumn, spring, and summer) in organic matter metabolism by microbial communities in open and buried reaches of three urban streams in Cincinnati, OH. We characterised DOM quality using fluorescence spectroscopy and extracellular enzyme profiles, and we measured the respiration response to carbon supplements in nutrient diffusing substrata (NDS). We hypothesised: (1) that algal production would lead to higher quality DOM in spring compared to other seasons and in open compared to buried reaches, (2) lower reliance of microbial respiration on recalcitrant carbon sources in spring and in open reaches, and (3) that microbial respiration would increase in response to added carbon in autumn and in buried reaches.
Several fluorescence metrics showed higher quality DOM in spring than autumn, but only the metric of recalcitrant humic compounds varied by reach, with more humic DOM in open compared to buried reaches. This likely reflected open reaches as an avenue for direct terrestrial inputs from the riparian zone.
Extracellular enzyme assays showed that microbes in buried reaches allocated more effort to degrade recalcitrant carbon sources, consistent with a lack of labile carbon compounds due to limited photosynthesis. Nitrogen acquisition enzymes were highest in autumn coincident with riparian leaf inputs to the streams. Buried and open reaches both responded more strongly to added carbon in autumn when terrestrial leaf inputs dominated compared to the spring when vernal algal blooms were pronounced.
Our data show that stream burial affects the quality of the DOM pool with consequences for how microbes use those carbon sources, and that heterotrophic respiration increased on carbon-

supplemented NDS in buried and open stream reaches in both seasons. Different carbon quality and use patterns suggest that urban stream infrastructure affects spatiotemporal patterns of bacterial respiration, with likely consequences for nitrogen and/or phosphorus cycling given that carbon use drives other biogeochemical cycles. Management actions that increase light to buried streams could shift the balance between allochthonous and autochthonous DOM in urban streams with consequences for spatiotemporal patterns in bacterial metabolism.

ORD-021631	Mosley, J., Ekman, D., Cavallin, E., Villeneuve, L., Ankley, G., Collette, T.. 2017. High-Resolution Mass Spectrometry of Skin Mucus for Monitoring Physiological Impacts and Contaminant Biotransformation Products in Fathead Minnows Exposed to Wastewater Effluent. ENVIRONMENTAL TOXICOLOGY AND CHEMISTRY, doi: 10.1002/etc.4003	EMMD	Peer Reviewed	CSS 17.01.01

Impact / Purpose Statement
Published in journal, Environmental Toxicology and Chemistry.

Product Description / Abstract
High-resolution mass spectrometry is advantageous for monitoring physiological impacts and contaminant biotransformation products in fish exposed to complex wastewater effluent. We evaluated this technique using skin mucus from male and female fathead minnows (Pimephales promelas) exposed to control water or treated wastewater effluent at 5%, 20%, and 100% levels for 21 d, using an onsite, flow-through system providing real-time exposure. Both sex-specific and non-sex-specific responses were observed in the mucus metabolome, the latter suggesting the induction of general compensatory pathways for xenobiotic exposures. Altogether, 85 statistically significant treatment-dependent metabolite changes were observed out of the 310 total endogenous metabolites that were detected (156 of the 310 were annotated). Partial least squares regression models revealed strong covariances between the mucus metabolomes and upregulated hepatic mRNA transcripts reported previously for these same fish. These regression models suggest that mucus metabolomic changes reflected, in part, processes by which the fish biotransformed xenobiotics in the effluent. In keeping with this observation, we detected a phase II transformation product of bisphenol A in the skin mucus of male fish. Collectively, these findings demonstrate the utility of mucus as a minimally invasive matrix for simultaneously assessing exposures and effects of environmentally relevant mixtures of contaminants.

ORD-022844	Sallam, M., Fizer, C., Pilant, A., Whung, P.. 2017. Systematic Review: Land Cover, Meteorological, and Socioeconomic Determinants of Aedes Mosquito Habitat for Risk Mapping. INTERNATIONAL JOURNAL OF ENVIRONMENTAL RESEARCH AND PUBLIC HEALTH. 14(10), 1230; doi:10.3390/ijerph14101230	SED	Peer Reviewed	SHC 1.62.1

Impact / Purpose Statement
Published in the International Journal of Environmental Research and Public Health.

Product Description / Abstract

Asian tiger and yellow fever mosquitoes (Aedes albopictus and Ae. aegypti) are global nuisances and are competent vectors for viruses such as Chikungunya (CHIKV), Dengue (DV), and Zika (ZIKV). This review aims to analyze available spatiotemporal distribution models of Aedes mosquitoes and their influential factors. A combination of five sets of 3–5 keywords were used to retrieve all relevant published models. Five electronic search databases were used: PubMed, MEDLINE, EMBASE, Scopus, and Google Scholar through 17 May 2017. We generated a hierarchical decision tree for article selection. We identified 21 relevant published studies that highlight different combinations of methodologies, models and influential factors. Only a few studies adopted a comprehensive approach highlighting the interaction between environmental, socioeconomic, meteorological and topographic systems. The selected articles showed inconsistent findings in terms of number and type of influential factors affecting the distribution of Aedes vectors, which is most likely attributed to: (i) limited availability of high-resolution data for physical variables, (ii) variation in sampling methods; Aedes feeding and oviposition behavior; (iii) data collinearity and statistical distribution of observed data. This review highlights the need and sets the stage for a rigorous multi-system modeling approach to improve our knowledge about Aedes presence/abundance within their flight range in response to the interaction between environmental, socioeconomic, and meteorological systems.

Submitted

ORD-022914	Berhane, T., C. Lane, Q. Wu, O. Anenkhonov, V. Chepinoga, B. Autrey, and H. Liu. Comparing pixel- and object-based approaches in effectively classifying wetland-dominated landscapes. Remote Sensing.	SED	Peer Reviewed	N/A

Impact / Purpose Statement
Submitted to the journal, Remote Sensing.

Product Description / Abstract
Wetland ecosystems straddle both terrestrial and aquatic habitats, performing many ecological functions directly and indirectly benefitting humans. Yet global wetland losses are substantial. Satellite remote sensing and classification informs wise wetland management and monitoring. Both pixel- and object-based classification approaches using parametric and non-parametric algorithms may be effectively used in describing wetland structure and habitat, but which approach should one select? We conducted both pixel- and object-based image analyses (OBIA) using parametric (ISODATA and maximum likelihood, ML) and non-parametric (random forest, RF) approaches in the Barguzin Valley, a large wetland (~500 km2) in the Lake Baikal, Russia, drainage basin. Four Quickbird multispectral bands plus various spectral metrics (e.g., texture, non-differentiated vegetation index, etc.) were analyzed using 142 field-based regions of interest sampled to characterize an in initial 18 ISODATA-based classes. We found the greatest accuracy using OBIA with RF approach (99.2%, segmentation scale 15) followed by pixel-based RF (98.5%) and pixel-based ML (94.2%), all using a six-layer stack (bands 1 to 4, texture, and elevation). Parsimoniously using just four bands in the pixel-based analyses resulted in high accuracy, 92.1% with pixel-based ML and 96.4% with pixel-based RF. Increasing the segmentation scale in the OBIA and RF approach (from 15 to 30, 50, and 100 pixels per object) decreased overall accuracy from 99.2% to 98.2%, 96.0%, and 88.7%, respectively. Quickbird band 4 (near-infrared, 760-900 µm) was the most important band for class discrimination. The greatest accuracy across 18

wetland classes was found with OBIA and RF, and in many cases image-objects may be of paramount importance. However, the OBIA approach requires substantial user input and resources (e.g., segmentation scale, object weights for compactness, etc.). Hence, we conclude that the random forest algorithm coupled with either an OBIA or pixel-based analysis is most useful in classifying wetland habitats.

ORD-023391	He, J., K. Alapaty, J. Herwehe, and R. Bullock. Studying Precipitation Partitioning in Multiscale Weather Forecasts: Impacts of Stability Restoration Methods. American Meteorological Society Monthly Weather Review.	SED	Peer Reviewed	ACE CIVA-1.1

Impact / Purpose Statement

Submitted to the journal, American Meteorological Society Monthly Weather Review.

Product Description / Abstract

Accuracy of environmental modeling studies can depend on the accuracy of meteorological inputs such as precipitation and related parameters. One important parameter in precipitation modeling is the convective adjustment timescale (τ) used in parameterized cumulus clouds to restore atmospheric stability. In this work, a generalized and simple stability restoration method for estimating τ is proposed for use in any convection parameterization scheme for shallow and deep clouds with direct links to the boundary layer. This new method and two other existing methods were tested to study precipitation biases and their partitioning (1) at different grid spacing for short term weather simulations; and (2) in longer term simulations using 12-km grid spacing for statistical performance evaluation for a warm period.

Results from the short term weather forecasts indicate that, as compared to the other two τ methods, our new method (1) improves temporal and spatial variations of precipitation in many regions; (2) grid-scale precipitation dominates over subgrid-scale precipitation as grid spacing decreases from 36- to 4-km grid spacing; and (3) at 4-km grid spacing the new τ produced the lowest subgrid-scale precipitation with the best precipitation estimates. In the longer term simulations using 12-km grid spacing, precipitation partitioning was affected by the three stability restoration methods. The new method produced the best subgrid-scale precipitation fraction patterns while its statistical performance suffered for total precipitation amount as compared to one of the other two methods that produced the best statistics for total precipitation but exhibited the largest overprediction of subgrid-scale precipitation.

ORD-023603	Luecken, D., S. Napelenok, M. Strum, R. Scheffe, and S. Phillips. Sensitivity of ambient atmospheric formaldehyde and ozone to precursor species and source types across the U.S.. International Journal of Environmental Science and Technology.	CED	Peer Reviewed	N/A

Impact / Purpose Statement

Submitted to the International Journal of Environmental Science and Technology.

Product Description / Abstract

Formaldehyde (HCHO) is an important air pollutant from both an atmospheric chemistry and human health standpoint. This study uses a photochemical Air Quality Model, CMAQ-DDM, to identify the sensitivity of HCHO concentrations across the US to major source types and hydrocarbons. In July, biogenic sources of hydrocarbons contribute the most to HCHO sensitivity, split between isoprene and other alkenes. Among anthropogenic sources, mobile sources of hydrocarbons and nitrogen oxides (NOx) dominate. In January, HCHO is more sensitive to anthropogenic hydrocarbon sources than biogenic sources, with mobile sources and residential wood combustion as large contributors. While ozone (O3) is 3 times more sensitive to NOx than hydrocarbons across most of the US., HCHO is 6 times more sensitive to hydrocarbons than NOx. In winter, both HCHO and O3 show negative sensitivity to NOx (increases with removal of NOx), although O3 increases are much larger. The relative sensitivities do not change substantially across different regions of the country.

ORD-022905	McEachran, A., K. Mansouri, S. Newton, B. Beverly, J. Sobus, and A. Williams. A Comparison of Three Chromatographic Retention Time Prediction Models. TALANTA.	EMMD	Peer Reviewed	CSS 18.01.01

Impact / Purpose Statement

Cleared by NCCT.
Submitted to the journal, Talanta.

Product Description / Abstract

High-resolution mass spectrometry (HRMS) data has revolutionized the identification of environmental contaminants through non-targeted analysis (NTA). However, chemical identification remains challenging due to the vast number of unknown molecular features typically observed in environmental samples. Advanced data processing techniques are required to improve chemical identification workflows. The ideal workflow brings together a variety of data and tools to increase the certainty of identification. One such tool is chromatographic retention time (RT) prediction, which can be used to reduce the number of possible suspect chemicals within an observed RT window. This paper compares the relative predictive ability and applicability to NTA workflows of three RT prediction models: (1) a logP (octanol-water partition coefficient)-based model using EPI SuiteTM logP predictions; (2) a commercially available ACD/ChromGenius model; and, (3) a newly developed Quantitative Structure Retention Relationship model called OPERA-RT. Models were developed using the same training set of 78 compounds with experimental RT data and evaluated for external predictivity on an identical test set of 19 compounds. Both the ACD/ChromGenius and OPERA-RT models outperformed the EPI SuiteTM logP-based RT model (R2=0.81-0.92, 0.86-0.83, 0.66-0.69 for training-test sets, respectively). Further, both OPERA-RT and ACD/ChromGenius predicted 95% of RTs within a ± 15% chromatographic time window of experimental RTs. Based on these results, we simulated an NTA workflow with a ten-fold larger list of candidate structures generated for formulae of the known test set chemicals using the U.S. EPA’s CompTox Chemistry Dashboard (https://comptox.epa.gov/dashboard), RTs for all candidates were predicted using both ACD/ChromGenius and OPERA-RT, and RT screening windows were assessed for their ability to filter out unlikely candidate chemicals and enhance potential identification. Compared to ACD/ChromGenius, OPERA-RT screened out a greater percentage of candidate structures within a 3 minute RT window (60% vs. 40%) but retained fewer of the known

chemicals (42% vs. 83%). By several metrics, the OPERA-RT model, generated as a proof-of-concept using a limited set of open source data, performed as well as the commercial tool ACD/ChromGenius when constrained to the same small training and test sets. As the availability of RT data increases, we expect the OPERA-RT model’s predictive ability will increase.

ORD-023764	Nguyen , T., P. Westerhoff , E. Furlong, D. Kolpin, A. Batt, H. Mash, K. Schenck, J.S. Boone, J. Rice, and S. Glassmeyer. Trends Between Modeled DeFacto Reuse and Analyzed Grab Samples for Contaminants of Emerging Concern at Water Treatment Plants in The USA. JOURNAL OF THE AMERICAN WATER WORKS ASSOCIATION.	SED	Peer Reviewed	SSWR 6.02B

Impact / Purpose Statement
Submitted to the Journal of the American Water Works Association.

Product Description / Abstract
Discharge of wastewater upstream of drinking water intakes is a potential source of contaminants of emerging concern (CEC). Chemically analyzed grab samples and De Facto Reuse in our Nations Consumable Supply (DRINCS) geospatial watershed modeling were used quantify CEC exposures at 22 surface water DWTP intakes with the aim of qualitatively comparing exposure risks obtained by the two approaches. Between 9 to 71 organic CECs were detected in grab samples. Geospatial analysis determined that 3 DWTPs had no upstream WWTP discharges, while several DWTPs had hundreds to over 1000 upstream WWTP discharges; DRINCS modelled de facto reuse levels at the study locations ranged from 80% during lower streamflows. Good agreement between the number of chemicals and de facto reuse calculated by DRINCS model were observed and advances the validity of using DRINCS to identify locations of DWTPs for future sampling and treatment technology testing.

Presentations

ORD-021512	Bagley, M. Synthetic algae and cyanobacteria: Great potential but what is the exposure risk? Presented at 2017 ISES Annual Meeting, RTP, North Carolina, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	N/A

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Green algae and cyanobacteria (hereafter, algae) have the attractive properties of relatively simple genomes, rapid growth rates, and an ability to synthesize useful compounds using solar energy and carbon dioxide. They are attractive targets for applications of synthetic biology, as entrepreneurs seek to transform them into unicellular autotrophic “factories” for industrial chemical production, which could augment or potentially disrupt traditional production pipelines. Although initial genetic

modifications were focused on optimizing the harvest of ethanol and other biofuels, commercial ventures are diversifying and climbing the value chain into industrial chemicals, specialty chemicals, and pharmaceuticals. Fueled by breakthroughs in molecular engineering, genomics, informatics and computer aided design, synthetic biology ventures have advanced rapidly and introductions of new products have the potential to overwhelm regulators' ability to evaluate their associated environmental exposure risks. Ecologically, these exposure risks are likely to be most profound for open water algal culture ventures that lack the containment controls of closed systems. Ecological risk assessment for synthetic algae has some parallels with that of previous genetically modified organisms, but the greater scale of genomic changes presents new uncertainties that could greatly alter the risk calculus. In this talk, I will compare and contrast eco-evolutionary drivers of synthetic algae risk compared to previous genetically modified organisms and highlight key ecological exposure questions that must be evaluated for effective regulation.

ORD-023506	Bandyopadhyay, R., O. Kaplan, R. Araujo, R. Dodder, and B. Smith. FREIDA (Framework of Resources for modeling Energy/Environmental/Economic Impacts of Development and Advancements) in Ports: a portfolio of interactive information resources, and an illustrative energy sector analysis focusing on the US East Coast. To be presented at 7th IEEE Global Humanitarian Technology Conference (GHTC) 2017, San Jose, CA, USA, 10/19/2017 - 10/22/2017.	SED	Presentation	SHC 4.61.5

Impact / Purpose Statement

Cleared by NRMRL

Presented at the 7th IEEE Global Humanitarian Technology Conference (GHTC) 2017, San Jose, CA, USA, 10/19/2017 - 10/22/2017.

Product Description / Abstract

Coastal communities constitute ~40% of the total US population, and roughly 50% of the national GDP is attributed to socio-economic activities in these regions. Port system operations and related industries constitute a majority of the industrial activities occurring in the region. This paper presents preliminary results from our work on the development of "FREIDA in Ports": an interactive information resource and modeling framework for port communities, that may be used to enhance resilience to extreme weather events and enable sustainable development. Because of the complex nature of port activities and its interconnections with the social, political, economic and environmental aspects of the coastal communities, it is often very difficult to map out a comprehensive humanitarian adaptation plan for sustainable port and industrial operations in the region. The framework of information resources includes a broad range of agents and related data/modeling resources that could play a key role in building port communities resilient to natural disasters and environmental impacts of industrial operations in the region. A subsequent section explores possible policy recommendations, disaster management and pollution mitigation techniques that could be designed based on data organized via the information framework. The illustrative scenario analysis discusses the impacts of catastrophic

weather events on the US energy sector using US EPA's MARKAL model. Resulting impacts on energy generation mix, air emissions, and energy prices are presented in detail, in addition to a detailed outline of the modeling technique, and a summary of the overall results.

ORD-021449	Barros, N., N. Tulve, D. Heggem, and K. Bailey. A Review of Stressors from the Built and Natural Environments Impacting American Indian Children's Health and Well-Being. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.1

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Exposures to chemical and non-chemical stressors from children’s environments during early development may contribute to differences in their health and well-being outcomes. Children from American Indian tribes may have a disproportionate burden of these stressors from their man-made (i.e., built environment) and natural surroundings. Our objective was to identify stressors from the built and natural environments that may affect the health and well-being of American Indian children. Databases (ProQuest, PubMed, Web of Science) were searched with key words and search strings (e.g., Alaska Native child) to identify scholarly literature focused on stressors, exposures, and health and well-being for American Indian children. A total of 2,535 references were identified. References were then excluded if they did not discuss American Indian children or were not the primary cohort of interest; discussed Tribes outside the U.S.; described interventions; or did not provide information about stressors from the built or natural environments. Of the 23 remaining references 10 discussed stressors from the built environment and 13 from the natural environment. For the built environment, the main stressors were poor indoor air quality from a wood stove, mold, or dust; lack of plumbing; dirt floors; and overcrowding. For the natural environment, however, only chemical stressors were identified, focusing on maternal and adolescent exposures to persistent organic pollutants and metals around hazardous waste sites (through contaminated waterways) and abandoned mines. Preliminary findings identified a limited number of studies (<30), demonstrating a major information gap. Analyses provide preliminary information about the nature of chemical and non-chemical stressors from built and natural environments that may influence American Indian children’s health and well-being, which may be distinct from other communities. Further analyses will be reported.

ORD-021326	Baxter, L., K. Dionisio, P. Pradeep, and L. Neas. Do Differences in Exposures Explain the Observed Heterogeneity in PM2.5 - Mortality Associations across U.S. cities?. To be presented at Annual Conference of the International Society of Exposure Science, Research Triangle Park, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	ACE PEP-1.4

Impact / Purpose Statement

Cleared by NHEERL.

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

This analysis evaluates exposure factors as potential determinants of the heterogeneity in city-specific associations between PM2.5 and mortality. Exposure factor variables were created based on housing characteristics, commuting patterns, heating fuel usage, and climatic factors data from national surveys. When survey data was not available, air conditioning (AC) prevalence was predicted utilizing machine learning techniques. We examined the heterogeneity in 312 city-specific PM2.5-mortality health effect estimates using inverse variance weighted linear regression with inverse variance weights. Prevalence of central AC predicted via machine learning techniques showed a strong relationship (R2 = 0.78) with the observed prevalence in surveyed cities. The national estimate (0.96% increase in total non-accidental mortality for a 10 µg/m3 increment in PM2.5 at lag 1) decreased by 0.12% (95% confidence interval (CI) -0.27 to 0.03) for an interquartile increase in the predicted prevalence of central AC. The other determinants examined were also found to modify the PM2.5-mortality association to varying degrees: median house size (+0.09%, 95% CI 0.01 to 0.18, for a 1 room increase in the median number of rooms), percentage of heating fueled by oil (+ 0.15%, 95%CI 0.10 to 0.20, for a percentage point increase), and heating degree days (HDD) (+0.31%, 95% CI 0.12 to 0.50, for a 1 day increase). In our analysis, the health impact of PM2.5 on mortality increases in cities with larger homes, more heating fueled by oil, more HDD, and less central AC.

ORD-021256	Benson, K., A. Grober, J. Truhe, K. Scruton, S. Williams, R. Helverson, P. Young, K. Thomas, M. Morgan, C. Croghan, and E. Irvin-Barnwell. A multi-site recycled tire crumb rubber characterization study: recruitment strategy and field sampling approach. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.62.2

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Recently, concerns have been raised by the public about the safety of tire crumb rubber infill used in synthetic turf fields. In response, the 2016 Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds (FRAP) was developed to examine key environmental and human health questions resulting from the use of tire crumb rubber. One specific objective of the FRAP was to characterize the chemicals, potential emissions, and toxicity of tire crumb rubber.

The goal of the tire crumb characterization study was to analyze new and aged/used tire crumb rubber for a variety of chemicals and to characterize field use patterns and maintenance procedures using a structured questionnaire. The aim was to recruit and sample 40 synthetic turf fields with tire crumb rubber infill. Ten fields in each of the 4 U.S. census regions were targeted. We used a convenience sampling approach for recruitment and online search engines to locate contact information for potential fields. Study inclusion criteria included a maximum of two outdoor fields per facility with fields having different installation years or different installation companies. In addition, we recruited tire recycling/crumb rubber manufacturing facilities located across the U.S.

A total of 306 community field owners/managers were contacted for potential participation. Sample collection was completed at 40 synthetic turf fields, including 21 community fields and 19 military installation fields. The final field count per census region was 9 Northeast fields (5 outdoor, 4 indoor), 13 South fields (11 outdoor, 2 indoor), 8 Midwest fields (2 outdoor, 6 indoor) and 10 West fields (7 outdoor, 3 indoor). Additionally, samples were collected at nine tire recycling/crumb rubber manufacturing plants across the country, including both ambient and cryogenic processes. Recruitment challenges will be discussed and field use and maintenance characteristics will be summarized.

ORD-021455	Brandon, N., K. Dionisio, K. Isaacs, D. Kapraun, R. Tornero-Velez, W. Setzer, and P. Price. Characterizing Exposure-Related Behaviors Using Agent-Based Models Embedded with Needs-Based Artificial Intelligence. Presented at 2017 ISES Annual Meeting, RTP, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 18.03.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Information on where and how individuals spend their time is important for characterizing exposures to chemicals in consumer products and in indoor environments. Traditionally, exposure assessors have relied on time-use surveys in order to obtain information on exposure-related behavior. In lieu of using surveys, we create an agent-based model (ABM) that is able to simulate longitudinal patterns in human behavior. By basing our ABM upon a needs-based artificial intelligence (AI) system, we create autonomous agents that mimic human decisions on residential exposure-relevant behaviors. The model predicts the behavior patterns for the following actions: sleeping, eating, commuting, and working/schooling. The model uses four different types of agents parameterized to represent the following U.S. demographic groups: working adults, non-working adults, school-aged children, and pre-school children. The parameters for the model are calibrated using survey data from the US Environmental Protection Agency’s Consolidated Human Activity Database (CHAD). The results demonstrate that the ABM can capture both inter-individual and intra-individual variation in the aforementioned behaviors as well as providing a needs-based rational as to how decisions on one’s behavior can affect subsequent behaviors. A key advantage of the needs-based AI is the possibility to synthesize plausible time-activity diaries de novo where this information is absent. We propose that by simulating human behavior, this ABM may allow exposure-assessors and other scientists to characterize exposure-related behavior quicker and in ways not possible with traditional survey methods.

ORD-023823	Bray, C., M. Strum, H. Simon, L. Riddick, M. Kosusko, and V. Rao. Assessment of important SPECIATE Profiles in EPA’s Emissions Modeling Platform and Current Data Gaps. Presented at 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	SED	Poster	N/A

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

The US Environmental Protection Agency (EPA)’s SPECIATE database contains speciation profiles for both particulate matter (PM) and volatile organic compounds (VOCs) that are key inputs for creating speciated emission inventories for air quality modeling. The objective of this work is to identify the most influential profiles based on mass and reactivity for various regions of the US. These profiles will be further investigated to characterize the profile quality and determine whether current matching between profiles and source types appropriately captures source type and regional variability in speciation. In cases where this analysis identified either low quality or poorly matched profiles, an in depth review of the SPECIATE database and the literature will be conducted to identify currently available suitable replacements. In cases where no suitable replacement profiles are found, this analysis will identify important gaps in the current literature which may be used to prioritize future speciation source testing. Through this process we aim to identify critical research needs, improve the SPECIATE database and improve a critical input for photochemical modeling efforts.

ORD-021517	Breen, M., S.Y. Chang, S. Arunachalam, V. Isakov, and R. Devlin. Modeling Air Pollution Exposure Metrics for the Coronary Artery Disease and Environmental Exposure (CADEE) Health Study. Presented at 2017 ISES Annual Meeting, Durham, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	ACE PEP-1.7

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Air pollution health studies often use outdoor concentrations from a central-site monitor as exposure surrogates. To improve exposure assessments, we previously developed and evaluated an exposure model for individuals (EMI), which predicts five tiers of individual-level exposure metrics for ambient air pollutants using outdoor concentrations, questionnaires, weather, and time-location information. We linked a mechanistic air exchange rate (AER) model to a mass-balance air pollutant infiltration model to predict residential AER (Tier 1), infiltration factors (Finf, Tier 2), indoor concentrations (Cin, Tier 3), personal exposure factors (Fpex, Tier 4), and personal exposures (E, Tier 5) for ambient air pollutants. In this study, we developed a novel model, called Exposure Tracker (ETrac), which extends EMI by including: (1) an air quality model to predict hourly census-block outdoor concentrations for four pollutants (PM, NOX, CO, EC), (2) a GPS-based microenvironment tracker (MicroTrac) model to predict time spent by individuals in various microenvironments. Using ETrac, we predicted daily exposure metrics (Tiers 1-5) for the 15 participants across 10 consecutive weeks in a cohort health study in central North Carolina called Coronary Artery Disease and Environmental Exposure (CADEE). Our modeled predictions for a total of 708 participant-days showed substantial house-to-house and temporal variability of AER, Finf, and Cin (Tiers 1-3); and subject-to-subject variability of Fpex and E (Tiers 4-5) for the four pollutants. The capability of ETrac could help reduce uncertainty of ambient pollutant exposure metrics used in health studies, such as CADEE, in support of improving health risk estimates.

ORD-023941	Campbell, P., J. Bash, C. Nolte, T. Spero, E. Cooter, and H. Pye. Impacts of Future Climate, Emission, and Land Use Changes on Aerosols and Air Quality over the Continental. Presented at 2017 AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	CED	Poster	ACE AIMS-2.2

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

Changes in climate, emission, and land use in the U.S. over the next century are imminent. The response of geologic, biogenic, and anthropogenic aerosol to interactions between these changes, however, are more uncertain and difficult to quantify. To explore these interactions, a “one atmosphere” modeling system consisting of the WRF (Weather Research and Forecast) model used with the CMAQ (Community Multiscale Air Quality) model, and linked to agricultural cropping management and soil biogeochemical processes in the EPIC (Environmental Policy Integrated Climate) model, is used to simulate emissions, dynamic air-surface exchange of trace gases and aerosols, gas-phase chemistry, secondary aerosol formation, transport, and deposition. Significant advancements have been incorporated into the latest aerosol module in CMAQ that include updates to organic and inorganic aerosol formation and properties, as well as an improved physics-based windblown dust parameterization. To consistently represent climate, land use, and air quality changes in this work, we modify WRF version 3.8.1 to improve its linkage to CMAQ version 5.2, and apply the advanced and modified WRF/Noah-CMAQ-EPIC system to dynamically downscaled Community Earth System Model (CESM) climate simulations, regional emission projections, and regional land use changes to study the impacts on aerosol formation and concentration, and ultimately the potential future of U.S. air quality by 2045 - 2055 under the RCP4.5 scenario. Specifically, we explore the changes in (1) inorganic aerosol formation regimes (e.g., in response to ammonia- vs. nitrate-limited regime changes), (2) organic aerosol formation and concentration changes (e.g., in response to biogenic volatile organic compound emission changes), and (3) windblown dust concentrations (e.g., in response to soil moisture and land use changes). We aim to relate the sensitivity of changes in (1) – (3) to their dominant climate, emission, and land use impacts to help provide insight into beneficial air quality management and mitigation strategies in the future.

ORD-023560	Catron, T., D. Phelps, S. Keely, N. Brinkman, E. Anneken, A. Kvasnicka, C. Wood, S. Gaballah, and T. Tal. Exploring the role of host-associated microbiota as mediators of bisphenol chemical toxicity in zebrafish. To be presented at NC American Society for Microbiology, Raleigh, NC, USA, 10/21/2017 - 10/21/2017.	SED	Presentation	CSS 17.01.01

Impact / Purpose Statement

Cleared by NHEERL

Presented at the at NC American Society for Microbiology, Raleigh, NC, USA, 10/21/2017 - 10/21/2017.

Product Description / Abstract

Exposure to Bisphenol A (BPA), a widespread environmental contaminant, has been associated with adverse endocrine and neurodevelopmental effects. Growing public concern over the safety of BPA has resulted in swift replacement with a suite of alternatives that uniformly lack sufficient toxicity data. Because host-associated microbial communities play important roles in nervous system development and harbor the ability to bioactivate or detoxify xenobiotics, we hypothesized that developmental exposure to bisphenol compounds may influence microbiota structure and/or cause colonization-dependent neurotoxicity. To test this, a semi-static system was used to first expose conventionally colonized zebrafish to BPA, Bisphenol AF (BPAF), Bisphenol B (BPB), Bisphenol F (BPF), or Bisphenol S (BPS). The classic estrogen receptor agonist 17beta-estradiol (E2) was used as a positive control. At 10 days post fertilization (dpf) larvae were assessed for mortality and gross malformations, and a range of potencies was observed: BPAF > E2 > BPB > BPA > BPF > BPS. To evaluate potential chemical-dependent shifts in microbiota structure in 10 dpf conventionally colonized zebrafish, 16S rRNA gene sequencing was performed. Concentration-dependent disruption of microbiota was observed with exposure to BPA, BPF, and BPS, while exposure to E2, BPB, and BPAF, the three most overtly toxic compounds, did not alter microbiota structure. To assess whether neurobehavioral toxicity was mediated by microbiota, we exposed three cohorts of zebrafish to all six compounds: conventionally colonized, axenic (microbe-free), and axenic colonized with zebrafish facility water at 1 dpf. At 10 dpf, neurobehavioral effects were assessed using an established light/dark behavioral assay. Colonization-dependent hypoactivity was observed only with E2 exposure. While some bisphenol compounds caused neurobehavioral toxicity in one or more cohorts, the effect was not colonization-dependent. Overall, these data demonstrate that the least overtly toxic bisphenol compounds cause the most significant alterations in microbiota structure in 10 dpf zebrafish larvae. These differential chemical effects suggest that current hazard identification strategies have the potential to misestimate risk if interactions between chemicals and microbiota are not considered. This abstract does not necessarily reflect EPA policy.

ORD-021349	Clifton, M., D. Mills, X. Liu, and K. Thomas. Characterization of Semi-Volatile Organic Chemicals from Tire Crumb Rubber. To be presented at International Society of Exposure Science (ISES) Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Poster	SHC 2.62.2

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Recycled tire crumb rubber (TCR) is often used as infill material in synthetic turf playing fields as well as some playgrounds. Concerns have been raised about the safety of this material and a multi-agency Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds was developed to investigate key factors that could impact the environment and human health. Here we present work done to characterize semi-volatile organic compounds (SVOCs) from direct solvent extraction of TCR and airborne emissions experiments. A wide range of SVOCs (including PAHs, phthalates, and chemicals related to rubber manufacturing) were selected for targeted analysis. Solvent selection, extraction techniques, and instrument parameters were investigated in order to better understand the TCR material and to develop the methods and appropriate QAQC required for sample analysis. TCR samples were collected from nine tire recycling plants and 40 synthetic turf fields across

the U.S. and were divided into subsamples for characterization experiments. TCR and emissions samples collected on PUF were extracted with 1:1 acetone:hexane. Emissions experiments were conducted at 25ºC, 46 % Relative Humidity (RH) and 1 h-1 air change (ACH) rate, and 60ºC, 6.6 % RH, 1 h-1 ACH in 53 L dynamic emission chambers. Data were acquired for all samples using GC/MS/MS in MRM mode with a calibration range of 0.1-500 pg/µL. MQLs, which were derived based on accuracy of standards compared to the calibration curves, ranged from 0.1-10 pg/µL. Non-targeted analysis was also performed by acquiring data by GCMS in scan mode (50-550 m/z) and then deconvoluting and library matching the spectra to tentatively identify components. Data obtained from the SVOC analyses will be used in conjunction with the other analyses that were conducted as part of the Federal Research Action Plan to identify key TCR chemical constituents, aid exposure assessment, and inform future studies related to TCR exposure.

ORD-021424	Dionisio, K., K. Isaacs, K. Phillips, D. Lyons, N. Brandon, G. Glen, T. Hong, A. Varghese, R. Avanasi, J. Levasseur, H. Hubbard, D. Vallero, P. Egeghy, and P. Price. Human Exposure Model (HEM): A modular, web-based application to characterize near-field chemical exposures and releases. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 18.03.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The U.S. EPA's Chemical Safety and Sustainability research program is developing the Human Exposure Model (HEM) to assess near-field exposures to chemicals that occur in various populations over the entire life cycle of a consumer product. The model will be implemented as a web-based, modular system that will produce estimates of population distributions of chemical exposure by route and releases to the environment, with one intended use to support human health impact assessments in Life Cycle Impact Assessments (LCIAs). The model determines aggregate doses of thousands of chemicals from the use of over 300 categories of consumer products over one year. Fundamental components of the model included in the beta-HEM release (September 2017) are the Residential-Population Generator (RPGen), Human Behavior, product formulation, and Source-to-Dose modules.

The RPGen module generates synthetic populations, together with characteristics that may drive product use such as detailed demographic and residential information for each household. The Human Behavior module uses agent-based modeling to determine longitudinal patterns of macro activities (eating, sleeping, commuting, working, and ‘idle’ time) and a product usage scheduler to define the use of consumer products on each day. CPDat, a database of product composition and chemical functional use data, is used to generate empirical product formulations. The Source-to-Dose module uses these outputs and data on chemical properties to calculate doses (by chemical, route and product category) for each individual, and corresponding environmental releases. This model allows for evaluation of near-field chemical exposures and environmental releases from the use of consumer products for incorporation into LCIA and other chemical assessments.

ORD-021438	Dionisio, K., K. Phillips, A. Williams, A. McEachran, J. Sobus, P. Price, J. Wambaugh, and K. Isaacs. New chemical use databases to support interpretation and dissemination of non-targeted analysis exposure data. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Exposure to chemicals in consumer products has been identified as a significant source of human exposure. To predict such exposures, information about the ingredients and their quantities in consumer products is required, but is often not available. The Chemicals and Products Database (CPDat) has been developed under the U.S. EPA’s Chemical Safety and Sustainability research program to fill these data gaps by using information from publicly-available sources. CPDat currently includes qualitative and quantitative information on reported product ingredients (from Safety Data Sheets or ingredient lists) in addition to multiple use categorizations (general, chemical function, and consumer product uses). Further, the CPDat database has been integrated with the Computational Toxicology Chemistry Dashboard (https://comptox.epa.gov/dashboard), which allows for linking of the product-specific (e.g. ingredients, weight fraction, use category) information in CPDat with chemical-specific information (e.g. structure, properties) and toxicity data (e.g. high-throughput screening and animal studies) available through the Dashboard. These data can aid in the interpretation or classification of accurate masses or molecular formulae identified in non-targeted analysis (NTA) studies. The Dashboard contains tools for searching for candidate chemical structures by mass or formulae, allowing selection among possible structures via investigation of CPDat information and other dashboard data sources. CPDat and the Dashboard are being updated to contain information about chemicals tentatively identified or confirmed in products in targeted and non-targeted analytical studies by EPA or others. As the database grows, it will increase the information available for rapidly and defensibly 1) evaluating the results of NTA of environmental or biological media or consumer products/articles and 2) characterizing chemicals in consumer products and articles for use in exposure and risk evaluations.

ORD-021249	Duvall, R., R. Williams, D. Vallano, A. Polidori, B. Feenstra, V. Papapostolou, and S. Garvey. Mapping Fine Particulate Matter and Ozone in Southern California Using Low-Cost Sensor Technologies. To be presented at 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	EMMD	Abstract	ACE EM-3.1

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

The emergence of small, portable, low-cost air sensors has encouraged a shift from traditional monitoring approaches for air quality. Over the past years, EPA has been actively involved in the

development and testing of these emerging sensor technologies as well as promoting informed use, deployment, and interpretation of data. EPA, in an effort involving the South Coast Air Quality Management District (SCAQMD) Air Quality Sensor Performance Evaluation Center (AQ-SPEC), deployed custom-built sensor pods measuring fine particulate matter (PM2.5), ozone (O3), relative humidity and temperature at nine locations throughout Southern California from January to April 2017. Southern California is an ideal testing location as it often experiences elevated air pollutant levels resulting from gasoline and diesel engines, ports, and industries. Meteorology (frequent sunny days and little precipitation) and geography also contribute to elevated pollution levels in the area. The goal of this project was to better understand performance and potential applications of low-cost sensors especially in the area of community monitoring. This presentation will highlight AQ-SPEC laboratory and field performance evaluations of the Citizen Science Air Monitor (CSAM) sensor pods designed and developed at EPA. In addition, this presentation will summarize the spatial and temporal variability of PM2.5 and O3 measurements collected at the monitoring locations which covered approximately a 200 km area in Southern California. This project will generate data that can be used to better understand air quality throughout the study area and provide the community with low-cost tools to measure air quality.

ORD-021364	Egorov, A., S. Griffin, R. Converse, J. Styles, E. Sams, A. Wilson, R. Baldauf, V. Isakov, L. Jackson, and T. Wade. Using health effect biomarkers to characterize benefits of urban green spaces. To be presented at International Society of Exposure Science (ISES), RTP, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.62.5

Impact / Purpose Statement

Cleared by NHEERL.

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Greater availability of urban green spaces has been linked to improved mental and physical health, and reduced mortality. Relative contributions of hypothesized pathways to improved health, such as relaxation and stress alleviation, enhanced physical activity, reduced exposure to air pollution, noise and heat, and beneficial exposure to natural allergens and microbes, remain to be characterized. The objective of an ongoing research project at US EPA is to characterize subtle biological changes associated with long-term exposure to green space using a panel of biomarkers of metabolic, neuroendocrine and immune function, and to produce novel information on pathways to health. A pilot cross-sectional study in the Durham-Chapel Hill, NC area used 1-meter resolution data on trees and herbaceous vegetation within 500 m of residences derived from the U.S. EPA EnviroAtlas land cover dataset. Eighteen health effect biomarkers were measured in serum or saliva samples from more than 200 adults. Regression models controlled for demographic covariates and spatial autocorrelation. Increased proportion of vegetated land cover (trees and grass) was associated with: 1) a highly significant reduction of a composite biomarker-based measure of physiological dysregulation known as allostatic load; 2) reduced odds of having potentially unhealthy levels of individual biomarkers associated with chronic inflammation and chronic stress; and 3) reduced odds of previously diagnosed depression. Ongoing analysis aims to characterize residential exposures of study participants to air pollutants and noise from local traffic using the Community LINE Source Model (C-LINE) developed by U.S. EPA and the University of North Carolina, and to assess potential effects of green barriers and green spaces in mitigating detrimental effects of gaseous and particulate air pollution on health biomarkers.

Further research efforts aim to evaluate associations between various measures of exposure to urban greenery, stress, physical activity, exposure to air pollutants, human microbiome, allostatic load and susceptibility to infectious and non-communicable diseases in prospective settings.

This abstract does not represent EPA policy.

ORD-022323	Egorov, A., S. Griffin, S. Fout, H. Ward, and T. Wade. Application of a salivary immunoassay to assess waterborne Cryptosporidium infections in a prospective community study. To be presented at Water and Health Conference, Chapel Hill, North Carolina, USA, 10/16/2017 - 10/20/2017.	SED	Abstract	SSWR 6.02D

Impact / Purpose Statement

Cleared by NHEERL

Presented at the Water and Health Conference, Chapel Hill, North Carolina, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

Background: Salivary antibody is a promising non-invasive biomarker of specific infections. This exploratory study used an in-house salivary immunoassay to assess waterborne transmission of Cryptosporidium.

Methods: Families with children were followed during summer-early winter periods in a Massachusetts city using a microbiologically contaminated river as its only source, before and after construction of a new water treatment plant. Monthly saliva samples (7,754 samples from 2,178 individuals) were analyzed for immunoglobulin (Ig) G responses to the recombinant protein gp15 protein of Cryptosporidium hominis using an in-house Luminex immunoassay. Immunoconversion was defined as at least four-fold increase in a ratio of anti-pathogen IgG response and total IgG with post-conversion response above the upper 90% prediction limit of spline function of age.

Results: Self-reported gastrointestinal illness during the previous month was associated with 2.9 (95% confidence limits 1.0; 8.5) adjusted odds ratio (aOR) of immunoconversion to Cryptosporidium. Swimming in natural water bodies or chlorinated pools during previous month was associated with 3.7 (1.2; 11.5) and 4.2 (1.4; 13.0) aORs of immunoconversion respectively. Analysis of interaction effect of self-reported non-boiled tap water consumption (dichotomized) and study phase demonstrated that drinking water from the municipal system was associated with 6.5 (1.4; 30.3) lower adjusted odds of Cryptosporidium immunoconversion after the introduction of new water treatment than before it.

Conclusion: Improved treatment of drinking water was associated with a significant reduction of transmission of Cryptosporidium through consumption of non-boiled tap water. Disclaimer: This abstract does not necessarily reflect EPA policy.

ORD-023914	Embry, M., T. Buckley, and R. Zaleski. Identifying Novel Data Sources to Refine Consumer Product Exposure Assessment: Multi-stakeholder Collaboration Addressing the Behavioral Data Gap in Consumer Product Chemical Exposure ?. Presented at 2017 Annual Meeting of ISES, Research Triangle Park, NC, USA, 10/16/2017 - 10/16/2017.	EMMD	Poster	CSS 18.03.01

Impact / Purpose Statement
Presented at the 2017 Annual Meeting of ISES, Research Triangle Park, NC, USA, 10/16/2017 - 10/16/2017.

Product Description / Abstract
The author did not submit an abstract

ORD-023851	Feinberg, S., R. Williams, G. Hagler, J. Low, L. Smith, R. Brown, D. Garver, M. Davis, M. Miller, J. Schaefer, J. Campbell, and T. McArthur. CitySpace Air Sensor Network: Evaluating Spatial Gradients of Urban Air Pollution with Low-Cost Air Sensor Technology. To be presented at 2017 American Association for Aerosol Research, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	EMMD	Presentation	ACE EM-1.3

Impact / Purpose Statement
Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract
Traditional air monitoring approaches, using regulatory monitors, have historically been used to establish regional-scale trends in air pollutants across large geographical areas. Recent advances in air pollution sensor technologies could provide additional information about nearby sources, support the siting of regulatory monitoring stations, and improve our knowledge of finer-scale spatiotemporal variation of ambient air pollutants and their associated health effects. Sensors are now being developed that are much smaller and lower-cost than traditional ambient air monitoring systems and are capable of being deployed in a nodal pattern to provide greater coverage of a given area. A recent significant sensor network implementation, the CitySpace project, was conducted by the US EPA and the Shelby County Health Department. A total of 16 solar and/or land powered sensor pods that collected one-minute time resolution data of particulate matter, wind direction and speed, temperature and humidity, were deployed across Memphis, TN for six months. The study began in October 2016 and involved local community review and support. The sensor pods were first deployed at the Shelby Farms NCore site to compare their measurements with a regulatory Tapered Element Oscillating Microbalance (TEOM) particulate monitor and establish sensor pod precision. The pods were then deployed at 16 locations throughout the city and surrounding area to develop a wireless sensor network with real-time data streaming capabilities (EPA’s VIPER network). The six-month deployment yielded a substantial data set, with on the order of 200,000 observations per parameter, per pod. After the monitoring period (March 2017), a selection of sensor pods was returned to the Shelby Farms site to evaluate potential

changes in sensor performance. Sensor pod pollutant data was normalized to regulatory TEOM data, based on the colocation periods, and used to develop comparisons between locations and explore the spatiotemporal variability of particulate pollution in the Memphis area.

ORD-021319	Frank, J. Meta-Analysis of Lead (Pb) in Multiple Environmental Media in the United States. To be presented at ISES 2017, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.6

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
The U.S. Environmental Protection Agency, Office of Research and Development, conducts probabilistic multimedia lead (Pb) exposure modeling to inform the development of health-based benchmarks for Pb in the environment. For this modeling, robust Pb concentration (level) data are needed for developing distributional model inputs. Objectives: To create a database of Pb levels measured in environmental media within the United States using data from published literature; and to summarize Pb levels by media type to refine model inputs. Methods: A systematic literature search was conducted to identify qualifying articles meeting specified criteria published from 1996 to early 2016. Article screening and database creation were reviewed independently by two researchers. A random effects model was used to summarize data by media type. Preliminary Results (reported as mean ± 95% CI for each single group summary): Residential (RES) soil samples (50±24 ppm) from non-urbanized areas (rural) were ~8x lower than urbanized RES areas (383±74 ppm). RES sites on or nearby Pb Superfund locations were largely classified as rural (8 of 9 sites) with soil Pb levels of 267±56 ppm. Schoolyard and playground soil Pb levels were 54±22 ppm. Community and RES garden soil Pb levels were 160±37 ppm. Soil Pb from non-RES Pb Superfund sites (1316±402ppm) were ~2x lower than soil collected at outdoor shooting ranges (3137±136 ppm). For air Pb, the results for sites classified as rural (0.0035±0.003 µg/m3) were ~5x lower than urbanized areas (0.0169±0.014 µg/m3). The results for Pb in drinking water for all areas reported in the literature was 2.25±1.79 ppb. Conclusions: The results from this analysis can inform future research and rule-making by providing insight into information gaps and key inputs in Pb multimedia modeling analyses, and by helping to identify potentially vulnerable groups. In addition, this information can be used to assess the effectiveness of remediation.

ORD-023825	Frank, J., A. Poulakos, and J. Xue. Meta-Analysis of Lead (Pb) in Multiple Environmental Media in the United States. Presented at 2017 ISES Annual Meeting, RTP, NC, USA, 10/15/2017 - 10/19/2017.	SED	Poster	SHC 2.63.6

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Introduction: The U.S. Environmental Protection Agency, Office of Research and Development, conducts probabilistic multimedia lead (Pb) exposure modeling to inform the development of health-based benchmarks for Pb in the environment. For this modeling, robust Pb concentration data are needed for developing distributional model inputs.

Objectives: To create a database of Pb levels measured in environmental media within the United States using data from published literature; and to summarize Pb levels by media type to refine model inputs.

Methods: A systematic literature search was conducted to identify qualifying articles meeting specified criteria published from 1996 to early 2016. Article screening and database creation were reviewed independently by two researchers. A random effects model was used to summarize data by media type.

Preliminary Results (reported as mean ± 95% CI for each single group summary): Residential (RES) soil samples (50±24 ppm) from nonurbanized areas (rural) were ~8x lower than urbanized RES areas (383±74 ppm). RES sites on or nearby Pb Superfund locations were largely classified as rural (8 of 9 sites) with soil Pb levels of 267±56 ppm. Schoolyard and playground soil Pb levels were 54±22 ppm. Community and RES garden soil Pb levels were 160±37 ppm. Soil Pb from non-RES Pb Superfund sites (1316±402ppm) were ~2x lower than soil collected at outdoor shooting ranges (3137±136 ppm). Air Pb reported in the literature for sites classified as rural (0.0035±0.003 µg/m3) were ~5x lower than urbanized areas (0.0169±0.014 µg/m3). The results for Pb in drinking water for all areas reported in the literature was 2.25±1.79 ppb.

Conclusions: The results from this analysis can inform future research and rule-making by providing insight into information gaps and key inputs in Pb multimedia modeling analyses, and by helping to identify potentially vulnerable groups. In addition, this information can be used to assess the effectiveness of remediation.

ORD-021292	Gardner, S., E. Heithmar, K. Kovalcik, G. Momplaisir, A. Williams, M. Medina-Vera, and T. Jones-Lepp. Multimodal Physicochemical Characterization of Tire Crumbs Used at Synthetic Turf Fields. To be presented at 27th International Society of Exposure Science Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Poster	2.2B

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

As part of a U.S. Federal Research Acton Plan to study possible environmental and human health implications of tire crumbs used as infill for synthetic turf, the Environmental Protection Agency (EPA) is evaluating the potential of human exposure to various chemicals from tire crumbs. Physicochemical characterization of tire crumbs from playing fields and from manufacturing plants, including minor- and trace-element composition, as well as particle size and general morphology, is fundamental to this

evaluation. EPA chose a multimodal approach to these characterizations: high resolution-inductively coupled plasma mass spectrometry (HR-ICPMS) for sensitive trace-element concentrations of sample digests; X-ray fluorescence (XRF) for minor- and trace-element characterization of individual particle size fractions without digestion; scanning electron microscopy (SEM) for size distributions and morphology of fine particles; and energy dispersive X-Ray spectrometry (EDS) for information on elemental composition of selected particles imaged by SEM. Samples for elemental measurements by HR-ICPMS were digested using a modified version of EPA method 3051a. Low detection limits and suppression of spectral interferences in complex matrices are benefits of HR-ICPMS. Particle Size Analysis (PSA) was performed on samples using sequential sieving. A floatation procedure was used to separate the sand from the crumb in samples with significant sand. A screening X-ray fluorescence analysis was performed on crumb size ranges separated during the PSA analysis, as well as on un-sieved samples. SEM imaging of fine particles was performed with a 24 keV electron beam and electron backscatter detection (BSD). Particles with significant non-carbon elemental composition were analyzed by EDS. This presentation describes the performance and demonstrates the complementary information provided by this multimodal physicochemical characterization of tire crumbs.

ORD-023835	Glen, G., H. Hubbard, J. Levasseur, P. Price, K. Dionisio, D. Vallero, and P. Egeghy. Residential and Population Generator (RPGen): Creating a detailed description of housing and occupants for predicting and describing chemical exposures. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 11.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The US EPA’s Human Exposure Model (HEM) is a modular stochastic model that simulates populations, assigns product use, and calculates direct and indirect exposure to consumer products. The Residential and Population Generator (RPGen) module of HEM randomly samples real-world data from the Public Use Microdata Sample (PUMS) data, the American Housing Survey (AHS) and the Residential Energy Consumption Survey (RECS) to create a simulated population of primary individuals together with their household structure and housing characteristics. The PUMS, AHS, and RECS databases are linked by housing type, region of the country, population density of location, household income, and by number of residents in a household and resident ages. Household characteristics were prioritized to those that impact exposure to consumer products and include the type of appliances, the number of cars, number of bathrooms, and size of house, among others. Household characteristics include the number of children, number of adults, and age and sex of each member. RPGen also assigns physiological variables to each primary individual using EPA’s “httk” R package.

Due to the modular structure of HEM, RPGen is a flexible tool for generating populations of humans and housing to fit a range of models and modeling needs. Currently, RPGen output drives an agent based model (ABM) module of HEM, which considers region, seasonality, and communal product use to develop the universe of consumer products to which the primary individual may be exposed. A series of rules based on demographic and housing characteristics further customize the consumer product use for

each household. After ABM schedules daily product use for all people in a household, HEM’s source-to-dose (S2D) module evaluates the direct and indirect exposures of each primary individual using a product use function for direct exposure, and a fugacity model to determine chemical residues that result in indirect exposure for all household members.

ORD-021446	Glen, G., H. Ozkaynak, H. Hubbard, J. Cohen, N. Tulve, L. Phillips, K. Thomas, and J. Moya. Using SHEDS-S/D to Estimate Soil and Dust Ingestion Rates for Children. Presented at 2017 ISES Annual Meeting, NC, Durham, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.8

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Soil and dust ingestion can be the primary pathway for environmental exposure to some pollutants. Studies have shown that young children, due to their greater mouthing behavior than older children or adults, are more vulnerable to incidental ingestion of soil and dust. However, available data to support the development of age-specific soil and dust ingestion rates are either limited or uncertain for most age groups. Our objective was to use the Stochastic Human Exposure and Dose Simulation Soil and Dust (SHEDS-S/D) model to estimate distributions of soil and dust ingestion rates for infants and children to determine if data gaps could be filled using this modeling approach.

We developed a new exposure scenario in SHEDS-S/D to capture exposures to indoor dust via pacifier use by infants and very young children. This exposure scenario accounts for the use of blankets or similar surfaces that may prevent direct contact of the pacifier with the floor. Although the inputs for this scenario were uncertain, the scenario was estimated to contribute approximately 20 mg/day to overall dust ingestion. We also conducted a sensitivity analysis by age group to determine key drivers of exposure. For infants and younger children, pacifier use drove exposure with the most sensitive variables being carpet dust loading, pacifier drop frequency, and the floor-to-pacifier transfer fraction. For older children, key variables were carpet dust loading, soil adherence, four hand properties, the frequency of hand-to-mouth contact, the area of the hand mouthed, the amount of floor contacted by the hand, and the fraction of dust removed by each hand-to-mouth event.

These results can be used to identify data limitations in developing robust soil and dust ingestion rates and to focus resources on the variables that will provide the most insight in developing age-specific rates, as well as describing differences in ingestion rates within and between populations.

ORD-021417	Glen, G., R. Avanasi, J. Levasseur, H. Hubbard, P. Price, and K. Isaacs. Characterizing use-phase chemical releases, fate, and disposal for modeling longitudinal human exposures to consumer products. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 18.03.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The US EPA’s Human Exposure Model (HEM) is an integrated modeling system to estimate human exposure to chemicals in household consumer products. HEM consists of multiple modules, which may be run either together, or independently. The Source-to-Dose (S2D) module in HEM uses a compartmental mass partitioning approach that models the release and transport of chemicals during product use as a series of stages including the initial use phase release, transfers during the use phase, end of the direct use phase, and direct exposure to residual chemicals. In the first stage, the fractional mass releases of chemicals that occur during the use of a product are determined for 11 possible compartments (indoor/outdoor air, indoor/outdoor surface, skin, gut, other body parts, solid waste, drain, appliance and retained solid product). The mass releases to each compartment vary by the type of product. Products are categorized into 17 different product categories based on the physical processes involved in their use (sprays, liquids, dusts etc.) and on their application location (body, indoor, outdoor surfaces, among others). The second stage determines the transfers between compartments during the time the product is used by processes such as, but not limited to, volatilization and settling. The third stage determines the movement of chemicals to household trash and residential waste water from wipe-off and rinse-off events. Some products have a fourth stage for modeling direct exposure to any residual chemical left on the skin or in the nearby area. The mass of chemicals in the indoor air and surface compartments at the end of the fourth stage are used as inputs to a fugacity module to determine the time series of post-use chemical concentrations in the home’s indoor air and surfaces. This approach allows for the efficient calculation of population-based residential human exposures and releases in support of mid-tier assessments and life-cycle analyses.

ORD-021468	Grossman, J., A. McEachran, A. Marcotte, A. Williams, and J. Sobus. Using Structural Similarity to Estimate Concentrations of Known Unknowns in Suspect Screening Analyses. To be presented at International Society of Exposure Science 27th Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Suspect screening analysis (SSA), based on high-resolution mass spectrometry (HRMS), has recently been adopted in environmental chemistry applications to enable broad-scale chemical surveillance and exposure monitoring. SSA is inherently a qualitative technique, and generally unable to provide quantitative information for a given compound in the absence of a conventional reference standard. Here, we introduce novel methodology that enables quantitation of known unknowns (i.e., HRMS features for which a probable structure can be put forth via identification algorithms and a custom SSA workflow) in samples without the use of conventional standards. Three blinded synthetic mixtures, based on US EPA ToxCast chemicals, were analyzed using liquid chromatography quadrupole time-of-flight mass spectrometry. Calibration curves were generated for tentatively identified compounds (via SSA), in the first two mixtures. SSA was then performed on the third mixture at multiple blinded dilutions. Molecular formulae were assigned to features in the third mixture and mapped to candidate

structures using the US EPA’s CompTox Chemistry Dashboard. Ranking/classification tools, along with novel semi-Data Dependent MS/MS methods, were used to propose and corroborate chemical structures for each formula. Chemical similarity coefficients were used to link candidate compounds from the third mixture to structurally-similar compounds with existing calibration data from the first two mixtures. Quantitation for each candidate compound, at each dilution, was performed using surrogate calibration curves, with a weighting scheme based on chemical similarity score (i.e., structurally-similar compounds were given more weight). The techniques described here allow for semi-quantitation of unknowns detected by SSA, and thus provide a means to generate exposure and dosage information to be considered in support of avant-garde chemical screening programs.

ORD-021585	Guiseppi-Elie, A. ISES Panel Discussion: Consumer Exposure Assessment: Tools and Information to Support a Fit-for-Purpose Approach to Exposure Risk Assessment. To be presented at ISES 2017, NC, RTP, USA, 10/15/2017 - 10/19/2017.	NERL IO	Abstract	N/A

Impact / Purpose Statement
Panel Discussion at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
The panel discussion can then consider areas such as future directions for consumer exposure science development – what are the focus areas and opportunities?

1. Overall

• Do we gain information by considering models within a fit for purpose framework?

• Are model roles or purposes clear?

• How does model purpose influence development?

2. Modeling Capabilities

• Are there opportunities to leverage approaches across models?

• How to take advantage of the full scope of tools available internationally?

• What are future areas for model development?

3. Model Input Data

• What are key model inputs and how might this data be obtained?

• Are there ways to better use emerging technologies that enable data collection?

• Do we need greater interaction with other disciplines? Social sciences, computational science?

ORD-021553	Guiseppi-Elie, A. Using 21st Century Exposure Science to Improve Risk Assessment. Presented at ISES 2017 Annual Meeting, RTP, NC, USA, 10/15/2017 - 10/19/2017.	NERL IO	Presentation	N/A

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Exposure science is used across the Federal government to inform many important actions. Federal agencies rely on exposure science or exposure assessments to allow them to develop risk mitigation strategies for public health and environmental concerns. The more precise these exposure assessments can be, the more targeted and in many cases, more limited the risk mitigation approaches can be. For example, EPA uses exposure science to more fully inform risk reduction strategies under the Toxics Substances Control Act (TSCA), the Clean Air Act (CAA) and other environmental statutes. To ensure state of the art exposure science, it is critical that exposure science approaches, tools and methodologies keep pace with emerging technologies, regulatory program requirements and societal needs. Major scientific advances in the field are needed to accomplish that goal. In 2010, the United States Environmental Protection Agency (EPA) and the National Institute of Environmental Health Sciences (NIEHS) commissioned the National Research Council (NRC) to develop a report with the goal of advancing exposure science, its use, and its impact similar to the NRC’s Toxicity Testing in the 21st Century: A Vision and a Strategy. This presentation will focus on the role of exposure science in decision-making, drawing on scientific advances, and how they enhance the risk assessment process. The presentation will highlight how recommendations from recent National Academies of Science reports, Exposure Science in the 21st Century: A Vision and a Strategy (2012) and Using 21st Century Science to Improve Risk-Related Evaluations (2016) bolster the premise that exposure science is critical in risk assessments.

ORD-021465	Guiseppi-Elie, A., A. Ragin-Wilson, E. Hooker, K. Thomas, E. Irvin-Barnwell, and J. Zambrana. The Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds - Background and Exposure Research Goals. To be presented at International Society of Exposure Science, Research Triangle Park, North Carolina, USA, 10/15/2017 - 10/19/2017.	NERL IO	Presentation	N/A

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Concerns have been raised by the public about the safety of recycled tire crumb rubber used in synthetic turf fields and playgrounds in the United States (U.S.). Several studies have been identified that examine potential exposure to tire crumb rubber infill in these settings. The existing studies do not comprehensively evaluate the potential exposures associated with these use scenarios. Additional research is needed to help fill important data gaps leading to improved exposure assessment for children and adults using synthetic turf fields and playgrounds with tire crumb rubber. In response, the U.S. Environmental Protection Agency (EPA), the Centers for Disease Control and Prevention/Agency for Toxic Substances and Disease Registry (CDC/ATSDR), and the U.S. Consumer Product Safety Commission (CPSC) launched a multi-agency federal research action plan to study key environmental human health questions associated with tire crumb rubber on synthetic turf fields and playgrounds. The “Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds” (referred to as the FRAP) was finalized in February 2016. The U.S. EPA and CDC/ATSDR prepared a research protocol to implement portions of the research activities outlined under the FRAP, including 1) conduct a literature review and data gaps analysis; 2) perform tire crumb rubber characterization, and 3) perform human exposure characterization for synthetic turf field users. CPSC is conducting research for assessing the potential risks to children associated with the use of recycled tire crumb rubber in playground surfaces. This presentation will provide the context for this exposure issue, an overview of the federal research efforts, and results of the literature review and data gaps analysis. The overall aim of these efforts to be presented will be to improve our understanding of child and adult exposures at fields and playgrounds with recycled tire crumb rubber.

ORD-021793	Hagler, G., D. Birkett, R. Henry, and E. Thoma. Back-trajectory modeling of high time-resolution air measurement data to separate nearby sources. To be presented at CMAS, Chapel Hill, NC, USA, 10/18/2017 - 10/20/2017.	RPDIS	Presentation	ACE PEP-1.5

Impact / Purpose Statement

Presented at CMAS, Chapel Hill, NC, USA, 10/18/2017 - 10/20/2017.

Product Description / Abstract

Strategies to isolate air pollution contributions from sources is of interest as voluntary or regulatory measures are undertaken to reduce air pollution. When different sources are located in close proximity to one another and have similar emissions, separating source emissions trends in situ is difficult. During 2012-2015, the EPA conducted the Region 2 Port-area Investigation of Emissions Reduction (R2PIER) project which collected 1-minute air quality and meteorological data at a site just south of the Port of Newark, New Jersey. This monitoring site was situated to maximize the ability to separate clustered sources, including the Port, the Newark International Airport, the New Jersey Turnpike, and other surrounding sources. Over three years, approximately 1.7 million measurements were made for PM2.5, sulfur dioxide (SO2), oxides of nitrogen (NO2, NO), carbon monoxide (CO), black carbon (BC), and local meteorology. New analytical approaches were developed to separate slowly varying from fast varying components of the time series, isolating the apparent component of the pollution time series attributable to local direct emissions. This separation indicated a significant component of the time series had a slowly varying characteristic, contributing a significant fraction of sulfur dioxide (43%), nitrogen oxides (56%), carbon monoxide (76%), particulate black carbon (59%), and particulate matter less than 2.5 micrometers in aerodynamic diameter (PM2.5, 73%). The direct emissions impacts isolated

from the time series were input, along with meteorology, into the Nonparametric Trajectory Analysis (NTA) model. The model results indicate that the highest or second highest average concentrations of these pollutants were associated with air that came from the Port of Newark. These Port-attributed concentrations decreased by up to ~50% during the study. The notable exception was PM2.5 which increased during the study period.

ORD-021596	Hashad, K., B. Yang, V. Isakov, and K.M. Zhang. Comparing different VIT formulations on near-road dispersion of particulate and gaseous pollutants. To be presented at 36th AAAR Annual Conf., Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	CED	Presentation	ACE PEP-2.5

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

Traffic-related air pollution is associated with a range of health issues including respiratory and cardiovascular problems, birth defects, and cancer. Recent studies suggest that the presence of roadside barriers can potentially mitigate exposure to air pollution for those living and working close to major roads. As vehicle-induced turbulence (VIT) has a strong effect on the initial dispersion of pollutants, it would be challenging to explore the impact of roadside barriers without a proper understanding of VIT. Our study compares three different techniques to model VIT. The first method models VIT as a fixed volume source where turbulence is uniformly produced in the highway computational domain. The second method treats each highway lane as a forcing zone where an estimate for the drag force produced by vehicles in that lane would be imposed into the domain. The third method distributes the drag force of each vehicle into the domain using a Gaussian function such that computational grid points close to vehicles would experience a strong forcing as opposed to grid point further away. To evaluate the accuracy of each method, the simulation results are compared to experimental data obtained in an USEPA field study on a major highway in Las Vegas. The experimental data include extensive, collocated measurements of traffic, turbulence and air pollutant concentrations. The turbulent kinetic energy and pollutant concentration obtained from the simulations are compared with those of the field study. The impact of VIT on pollutant dispersion will also be explored for the different techniques.

ORD-023658	Hibbert, K., M. Morgan, G. Grissom, and S. Utile. Athletes' Selected Micro-Activities on Turf Fields: Utilizing Extant Videography for Quantification of Events During Soccer, American Football, and Field Hockey Play. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.	SED	Poster	SHC 2.62.3

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Concerns have been recently raised about the potential exposures of athletes to chemicals when playing on synthetic turf fields. Previous research has shown that micro-activities (i.e., hand-to mouth and skin-to-surface contacts) are important factors in people’s exposures to chemicals in outdoor settings. However, no published data have been identified for exposure-related micro-activities of athletes engaged in various sports on synthetic turf fields needed for exposure modeling. The objective of this study was to quantify the frequency of micro-activity events of participants playing soccer, field hockey, and (American tackle) football on synthetic and natural turf fields from publicly-available videos. Using the social media website YouTube, extant videography was systematically mined for children and adults

playing soccer/field hockey or football for a minimum of 15-minutes or 10-minutes, respectively. A total of 60 players were identified playing soccer (children: n = 10; adults: n = 10), field hockey (children: n = 10; adults: n = 10), and football (children: n = 10; adults: n = 10). Videos were downloaded as mp4 files and viewed on a computer using Windows Media Player software. Trained technicians tallied on paper the frequencies of hand-to-mouth, object-to-mouth, hand-to-turf, and object-to-turf events of each athlete. Frequency events for each type of micro-activity were normalized to one hour per athlete. Preliminary results showed no significant differences in frequencies of micro-activities depending on type of field. Also, there were no significant differences for individual micro-activities by age (children vs. adults). ANOVA analysis revealed significantly higher (p < 0.001) hand-to-mouth, object-to-mouth, hand-to-turf, and body-to-turf events for football players compared to soccer and field hockey players. This information suggests that type of sport played may have greater impact on potential exposures to chemicals than age or field type.

ORD-021268	Hibbert, K., and N. Tulve. Review of Non-Chemical Stressors from the Social Environment. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	N/A

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Non-chemical stressors (e.g., noise, diet, temperature, overcrowding) are found in the built, natural and social environments. Correlations between exposure to non-chemical stressors in the social environment (e.g., SES, exposure to violence, acculturation) and negative health outcomes in children have been shown. Associations between exposure to chemical stressors and changes in children’s health have also been shown. What we need to better understand are the interrelationships between chemical and non-chemical stressors and children’s health. Children may be more vulnerable to exposures from stressors due to their developmental stage and lifestage-specific activities. Our objectives were to 1) review the state-of-the-science in regards to non-chemical stressors found in a child’s social environment and 2) rank and prioritize those stressors. A systematic review of non-chemical stressors found in a child’s social environment was completed. Combinations of search strings were entered into PubMed, Google Scholar, and PsychInfo. Inclusion criteria resulted in 372 articles and 678 non-chemical stressors. From these articles, data was extracted into a searchable database for statistical analysis. The review resulted in 11 categories of non-chemical stressors (acculturation, adverse childhood experiences, economic, education, food, greenspace, overcrowding, social support, stress, urbanization, and exposure to violence). Food,

economic, acculturation, and violence had more articles than other topic areas. Analysis of the topic areas suggested significant positive and negative associations with children’s health. In general, non-chemical stressors from the social environment are found in combination. Our analysis suggests that non-chemical stressors are associated with children’s health. Additionally, chemical and non-chemical stressors should be considered together when evaluating children’s health.

ORD-021245	Hibbert, K., M. Morgan, G. Grissom, and S. Utile. Athletes’ Selected Micro-Activities on Turf Fields: Utilizing Extant Videography for Quantification of Events During Soccer, American Football, and Field Hockey Play.. To be presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	N/A

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Concerns have been recently raised about the potential exposures of athletes to chemicals when playing on synthetic turf fields. Previous research has shown that micro-activities (i.e., hand-to-mouth and skin-to-surface contacts) are important factors in people’s exposures to chemicals in outdoor settings. However, no published data have been identified for exposure-related micro-activities of athletes engaged in various sports on synthetic turf fields needed for exposure modeling. The objective of this study was to quantify the frequency of micro-activity events of participants playing soccer, field hockey, and (American) football on synthetic and natural turf fields from publicly-available videos. Using the social media website YouTube, extant videography was systematically mined for children and adults playing soccer/field hockey or football for a minimum of 15-minutes or 10-minutes, respectively. A total of 60 players were identified playing soccer (children: n = 10; adults: n = 10), field hockey (children: n = 10; adults: n = 10), and football (children: n = 10; adults: n = 10). Videos were downloaded as mp4 files and viewed on a computer using Windows Media Player software. Trained technicians tallied on paper the frequencies of hand-to-mouth, object-to-mouth, hand-to-turf, and object-to-turf events of each athlete. Frequency events for each type of micro-activity were normalized to one hour per athlete. Preliminary results showed no significant differences in frequencies of micro-activities depending on type of field. Also, there were no significant differences for individual micro-activities by age (children vs. adults). ANOVA analysis revealed significantly higher (p < 0.001) hand-to-mouth, object-to-mouth, hand-to-turf, and body-to-turf events for football players compared to soccer and field hockey players. This information suggests that type of sport played may have greater impact on potential exposures to chemicals than age or field type.

ORD-023926	Hogrefe, C. Overview of the Air Quality Model Evaluation International Initiative (AQMEII). Presented at Teleconference of WG4 of NADP CLAD Science Committee, Teleconference, Teleconference, USA, 10/17/2017 - 10/17/2017.	CED	Presentation	ACE AIMS-1.4

Impact / Purpose Statement

Presented at a teleconference of WG4 of NADP CLAD Science Committee, Teleconference, Teleconference, USA, 10/17/2017 - 10/17/2017. 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

This presentation provides an overview of the Air Quality Model Evaluation International Initiative (AQMEII). It contains a synopsis of the three phases of AQMEII, including objectives, logistics, and timelines. It also provides a number of examples of analyses conducted through AQMEII with a particular focus on past and future analyses of deposition.

ORD-021522	Ingle, B., B. Veber, J. Nichols, J. Wambaugh, and R. Tornero-Velez. In Silico Prediction of Toxicokinetic Parameters for Environmentally Relevant Chemicals with Application to Risk-Based Prioritization. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 10.02

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Toxicokinetic (TK) models can help bridge the gap between chemical exposure and measured toxicity endpoints, thereby addressing an important component of chemical risk assessments. The fraction of a chemical unbound by plasma proteins (Fub) and metabolic clearance rate (CLint) are critical TK parameters, accounting for aspects of the distribution, metabolism and excretion that determine in vivo tissue concentrations. Yet, limited TK data are available for environmentally relevant chemicals, including approximately 8000 chemicals with in vitro bioactivity data collected by Tox21. Quantitative structure-activity relationships (QSAR) for Fub and CLint were developed with in vitro assay data for both pharmaceuticals and chemicals in the ToxCast screening initiative using machine learning algorithms and open source descriptors. The models were shown to offer reliable in silico predictions of Fub and CLint for a diverse array of chemicals within the applicability domains. Incorporating the QSARs into TK models allowed a high throughput risk-based prioritization scheme informed by the margin between bioactive doses and human exposure. These QSAR models aid in the identification and prioritization of those chemicals with the highest probability of triggering adverse outcomes.

ORD-021310	Irvin-Barnwell, E., K. Thomas, K. Benson, Z. Li, and A. Ragin-Wilson. Characterization of Exposure Potential during Activities on Synthetic Turf Fields with Recycled Tire Crumb Rubber Infill. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.62.2

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds (FRAP), released in February 2016, is a multi-agency research plan in response to concerns over the use of tire crumb rubber as infill on synthetic turf fields. The FRAP outlines specific research objectives, including characterizing tire crumb rubber and implementing a pilot-scale observational exposure characterization study.

In December 2016, ATSDR and the USEPA released a FRAP Status Report. The report included an in-depth literature review and data gaps analysis. Key data gaps included limited exposure information. Specifically, there was limited data on exposure factors, ingestion and dermal routes of exposure, and exposures to tire crumb particles. Additionally, biomonitoring data were very limited, and no epidemiological studies were identified. The Status Report also described tire crumb characterization activities. Data from the tire crumb characterization study is being used to identify key chemical and physical property information and to inform implementation of the exposure characterization study.

Data from the pilot-scale exposure characterization study, while limited, will allow for further exploration of activities and use patterns that could result in exposure to chemicals from the tire crumb rubber infill by children and athletes who have the potential for high-end exposures. Additionally, the data gained from the study will inform biomonitoring approaches for exposure assessment and elucidate the key information needs which would be required for the development of an epidemiological study.

The current presentation will focus on the exposure characterization component of the FRAP and how the ongoing activities, along with exposure information from previous studies, will be used to better characterize synthetic turf field user exposures and inform future research activities. An update on the exposure characterization study will be presented.

ORD-021422	Isaacs, K., C. Bevington, K. Phillips, A. McEachran, A. Williams, J. Wambaugh, and J. Sobus. Media-Specific Classification Models for Ranking Candidate Unknown Chemicals in Non-targeted Analyses. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Monitoring of chemicals in environmental and biological media can inform estimates of exposure for supporting possible regulatory decisions and mitigation strategies. New technologies are allowing for the increased use of high-throughput (HT) monitoring approaches based on high-resolution mass spectrometry. However, HT approaches such as non-targeted (NTA) and suspect-screening (SSA) analyses require additional methods for identifying unknown chemical analytes from observed masses or molecular formulae. Current approaches for identifying “known unknowns” in NTA have relied on ranking candidate structures by number of literature sources or chemical database references. We now augment these approaches with chemical-specific predictions of the likelihood that a chemical might be found in an environmental medium. We use supervised machine learning (ML) approaches to classify chemicals on the basis of their unique properties, structures, uses, or other

characteristics (collectively called “descriptors”). By analyzing a training set of chemicals known to be present or absent from a specific medium, the ML methods generate an empirical model that can be used to classify other chemicals. Here we develop ML models for likely media occurrence by analyzing chemicals previously identified in various environmental and biological media. The monitoring data, which were collected from public sources, were used to successfully generate 13 cross-validated medium-specific classification models, which can be used to predict probabilities of media occurrence for any unknown chemical. The models were applied to a set of chemicals that are poorly ranked using data-source based methods alone, and the value and limitations of the models for the purpose of chemical ranking in NTA were evaluated. The views expressed here are those of the authors and do not necessarily reflect the views or policies of the U. S. EPA.

ORD-021549	Isaacs, K., J. Wambaugh, P. Price, J. Bare, K. Dionisio, K. Phillips, W. Setzer, C. Barber, B. Wetmore, R. Tornero-Velez, J. Orme-Zavaleta, R. Thomas, E. Wong, and C. Fehrenbacher. Exposure Modeling Tools and Databases for Consideration for Relevance to the Amended TSCA (ISES). To be presented at ISES 2017, RTP, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The Agency’s Office of Research and Development (ORD) has a number of ongoing exposure modeling tools and databases. These efforts are anticipated to be useful in supporting ongoing implementation of the amended Toxic Substances Control Act (TSCA). Under ORD’s Chemical Safety for Sustainability Research Program, new databases of how chemicals are used in commerce (e.g., in products or industrial processes) have been collated from dozens of public resources. These use data have enabled the development and application of high-throughput (HT) pathway-specific exposure models (e.g. the HT Stochastic Human Exposure and Dose model) and calibrated consensus exposure predictions for thousands of chemicals evaluated with biomonitoring data. These tools allow identification of the potential route of chemical exposure for certain conditions of use. A newer effort, the Human Exposure Model, incorporates new information on population variability (e.g., demographics, product use, geography, housing) that impacts exposures, and thus may be applicable to the identification of potentially exposed or susceptible subpopulations. To provide context to these predictions, new HT methods are being developed for converting external exposures to internal tissue doses, including methods that incorporate physiologic and lifestage variability. Finally, human-oriented exposure models also provide chemical release input to new ecological exposure models, which are being evaluated with public water monitoring data. While the amended TSCA provides an opportunity for ORD exposure modeling tools and databases to support amended TSCA, prior to any implementation the fitness-for-purpose of these projects (e.g., for prioritization, scoping, or risk evaluation) must be evaluated in the context of TSCA requirements. The views expressed here are those of the authors and do not necessarily reflect the views or policies of the U. S. EPA.

ORD-021495	Isaacs, K., K. Dionisio, K. Phillips, J. Wambaugh, P. Price, and A. Guiseppi-Elie. Advancing Models and Data for Characterizing Exposures to Chemicals in Consumer Products. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

EPA’s Office of Research and Development (ORD) is leading several efforts to develop data and methods for estimating population chemical exposures related to the use of consumer products. New curated chemical, ingredient, and product use information are being collected from public sources including 1) chemical weight fractions (WFs) collected from Material Safety Data Sheets 2) WFs predicted from ingredient lists, 3) product use patterns developed from purchasing data and 4) chemical function data. The functional use data is also being used to develop chemical structure and/or property-based models for function and product weight fraction, which can aid in filling gaps in existing ingredient data. In addition, under the Exposure Forecasting (ExpoCast) project, high throughput (HT) analytical methods are being evaluated for characterizing the composition of different products, a potentially rich source of new data for modeling and evaluation. These new data streams can parameterize mechanistic models for use in both high-throughput chemical screening and prioritization and higher-tier applications such as targeted exposure assessments or chemical life-cycle impact evaluations. For chemical prioritization, ORD has developed the High Throughput Stochastic Human Exposure and Dose Simulation (SHEDS-HT) model, which predicts aggregate population exposures based on chemical WFs and use patterns in over 300 consumer product categories. A higher-tier model, the Human Exposure Model (HEM), is being developed to consider additional factors impacting variability in exposures and internal chemical concentrations, including physiological variability and demographic and longitudinal patterns in product use. HEM will incorporate agent-based models of product use derived from considering a “needs-based” (e.g., personal hygiene, pest control) framework. These data and models will improve the prediction of chemical exposures in support of risk-based decision making.

ORD-021582	Jaoui, M., J. Offenberg, M. Lewandowski, A. Holder, and T. Kleindienst. Characterization of Hydroxy/Carboxyl-Nitro Compounds in SOA from Aromatic Oxidation: Implication for PM2.5. To be presented at American Association for Aerosol Research (AAAR), Research Triangle Park, NC, USA, 10/16/2017 - 10/20/2017.	EMMD	Presentation	ACE AIMS-1.3

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

SOA generated in our laboratory in the past fifteen years from the photooxidation of aromatics/NOx systems were yellow to light brown compared to those generated from biogenic precursors. Literature review shows that compounds containing aromatic ring(s) and/or nitro group(s) formed through

atmospheric oxidation may potentially be responsible, in part, for the optical properties associated with ambient particles, therefore influencing aerosol radiative forcing.

In this study, an analytical technique developed previously in our laboratory for the identification and quantification of multifunctional compounds was extended to compounds containing at least one nitro group(s). This technique is based on silylation using BSTFA as derivatizing agent, followed by GC-MS analysis in EI and methane-CI modes. This approach was tested on standards and on SOA from photooxidation experiments of toluene, benzene, ethylbenzene, o/m/p-xylenes, m-cresol, catechol, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, naphthalene, 1-methylnaphthalene and 2-methylnaphthalene in the presence of NOX. This technique has the advantage for identifying unambiguously unknown organic compounds containing -OH/-COOH, and -NO2 group(s). For example, CI spectra contain ions at m/z (M.+ + 1), (M.+ + 29), (M.+ + 41), (M.+ - 15), (M.+ - 89), and 73 for compounds bearing only hydroxy/carboxylic groups and (M.+ - 31) for those bearing also nitro group(s). To determine the presence

of these compounds in the atmosphere, PM2.5 filters collected in Research Triangle Park, NC, USA during 2003 were re-analyzed using the same analytical technique. GC-MS analysis showed the occurrence of some of these potential light absorbing compounds in chamber SOA and ambient PM2.5, indicating the impact of aromatics on brown carbon. This work describes systematically a method for identifying multifunctional compounds containing one or more nitro/hydroxyl/carboxylic groups. This is a way of supplementing optical measurements with compound identification through established, tested, reliable GC-MS methods. This isn’t a stand-alone tool, it is part of a broad suite of tools intended to address a larger problem than just aerosol composition and its relationship to optical properties.

ORD-023897	Kilaru, V. Framework and Data Consideration to Advance Exposure Science. To be presented at 2017 ISES Conference, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.	EMMD	Presentation	ACE CIVA-3.1

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
The author did not submit an abstract

ORD-023897	Kilaru, V. Framework and Data Consideration to Advance Exposure Science. To be presented at 2017 ISES Conference, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.	EMMD	Presentation	ACE CIVA-3.1

Impact / Purpose Statement
Cleared by NHEERL

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

We previously demonstrated that, on a mass basis, lung toxicity associated with particulate matter (PM) from flaming smoke aspirated into mouse lungs is greater than smoldering PM. This finding however has to be validated in inhalation studies to better predict real-world exposures. Thus, we modified an existing combustion system to precisely control and maintain smoke concentrations during the combustion process. We generated biomass smoke from peat and eucalyptus fuels under smoldering and flaming phases for up to 1 hour, and measured PM and volatile organic compounds (VOCs) levels. Smoldering PM levels were ~10 times higher than flaming PM with carbon monoxide (CO) held at similar levels to equalize potentially interfering CO health effects. Mice were exposed by inhalation for 1 hour/day for 2 days and then assessed for lung toxicity at 4 and 24 h after the second exposure. PM levels were ~40 and ~4 mg/m3 under smoldering and flaming phases, respectively, while CO levels ranged from ~80 to 110 ppm for all exposures. Notably, VOCs/PM ratios were higher (up to 7 times) in flaming than smoldering smoke. Smoldering peat and eucalyptus smoke elicited significant inflammation (neutrophils) in mouse lungs at 4 h post-exposure while flaming smoke from either fuel caused even greater lung inflammation at 24 h post-exposure. Similarly, a significant increase in an index of airflow obstruction was observed in mice exposed to flaming peat and eucalyptus, and smoldering eucalyptus smoke immediately after each day of exposure. These results suggest that although flaming smoke contains much less PM mass than smoldering smoke, the health risk of this exposure is, on a mass basis, greater than that from smoldering emissions. These observations support the concept that health risks of smoke exposure vary depending on the type of fuel and combustion conditions. [This abstract does not represent EPA policy]

ORD-023976	King, M., J. Haglund, A. Kalbas, S. Beck, A. Zuniga, and P. Solomon. Performance Testing of Two Virtual Impactors (VI). To be presented at 2017 AAAR Meeting, Research Triangle Park, NC, USA, 10/19/2017 - 10/19/2017.	EMMD	Poster	ACE 143

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

To evaluate a newly designed inlet nozzle for virtual impactors expected to improve the collection efficiency and reduce wall losses for use in high and low volume samplers.

ORD-023976	King, M., J. Haglund, A. Kalbas, S. Beck, A. Zuniga, and P. Solomon. Performance Testing of Two Virtual Impactors (VI). To be presented at 2017 AAAR Meeting, Research Triangle Park, NC, USA, 10/19/2017 - 10/19/2017.	EMMD	Poster	ACE 143

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract
To evaluate a newly designed inlet nozzle for virtual impactors expected to improve the collection efficiency and reduce wall losses for use in high and low volume samplers.

ORD-021365	Koplitz, S., and C. Nolte. Implications of emission inventory choice for modeling fire-related pollution in the U.S.. Presented at 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/19/2017.	SED	Presentation	ACE CIVA-1.3

Impact / Purpose Statement
Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract
Fires are a major source of particulate matter (PM), one of the most harmful ambient pollutants for human health globally. Within the U.S., fire emissions can account for more than 30% of total PM emissions annually. In order to represent the influence of fire emissions on atmospheric composition, regional and global chemical transport models (CTMs) rely on fire emission inventories developed from estimates of burned area (i.e. fire size and location). Burned area can be estimated using a range of top-down and bottom-up approaches, including satellite-derived remote sensing and on-the-ground incident reports. While burned area estimates agree with each other reasonably well in the western U.S. (within 20-30% for most years during 2002-2014), estimates for the southern U.S. vary by more than a factor of 3. Differences in burned area estimation methods lead to significant variability in the spatial and temporal allocation of emissions across fire emission inventory platforms. In this work, we implement fire emission estimates for 2011 from three different fire emission products (NEI, FINN, and GFED4s) into the CMAQ regional air quality model to quantify and characterize differences in simulated fire-related PM and ozone concentrations across the contiguous U.S. due solely to the emission inventory used. Understanding the sensitivity of modeling fire-related PM and ozone in the U.S. to fire emission inventory choice will inform future efforts to assess the implications of present and future fire activity for air quality and human health at national and global scales.

ORD-022765	Krug, J., J. Offenberg, M. Colon, K. Docherty, B. Habel, and R. Long. Wintertime Submicron Particulate Matter in Logan, UT as Measured by SMPS and EPC. To be presented at AAAR 36th Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	EMMD	Abstract	ACE EM-1.6

Impact / Purpose Statement
Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract
Submicron particulate matter (PM) in the atmosphere is typically emitted directly or formed through secondary processes such as condensation and nucleation of semivolatile compounds, little submicron PM is generated by natural processes such as wind-blown dust. Submicron PM is not currently regulated

by the EPA beyond inclusion with the PM2.5 standard on a mass basis. There is significant interest in measurement of submicron PM for understanding exposure risks and potential health effects related to exposure. Because individual submicron particles have relatively little mass, particle number concentration could be the most relevant metric in health effects studies. Due to wintertime atmospheric inversions, Logan UT frequently experiences exceedances in PM2.5. To better understand the local submicron PM, concentrations were monitored by Scanning Mobility Particle Sizer (SMPS) and by Environmental Particle Counter (EPC) during January and February of 2017 at a field site located in Logan UT. Daily median particle diameter is reported as well as particle number concentrations as measured by the SMPS and EPC. Trends are examined for correlation of submicron PM concentration to local atmospheric inversion events.

ORD-023586	Kvasnicka, A., S. Gaballah, D. Phelps, T. Catron, N. Brinkman, S. Keely, E. Anneken, C. Wood, and T. Tal. Specific strains of bacteria are required for neurobehavioral development in zebrafish larvae. To be presented at NC American Microbiological Society, Raleigh, NC, USA, 10/21/2017 - 10/21/2017.	SED	Abstract	CSS 17.01.01

Impact / Purpose Statement

Cleared by NHEERL

Presented at the NC American Microbiological Society, Raleigh, NC, USA, 10/21/2017 - 10/21/2017.

Product Description / Abstract

There is an increasing appreciation of the relationship between gut microbiota and nervous system development and function. We previously showed that axenic (microbe-free) larvae are hyperactive at 10 days post fertilization (dpf) relative to colonized zebrafish larvae. Interestingly, while exposure to heat-killed bacteria or microbe-associated molecular patterns failed to block hyperactivity in axenic larvae, colonization of axenic larvae with Aeromonas veronii or Vibrio cholerae produced locomotor hypoactivity relative to colonized controls. These data suggest that there is a developmental requirement for certain types of microbes modulate host behavior. To address this hypothesis, eight bacterial isolates were obtained from 10 dpf conventionally colonized zebrafish larvae. 16S rRNA gene sequencing identified four unique gram-negative isolates: Acinetobacter, Vibrio, Comamonas, and Comamonadaceae. Colonization of axenic embryos at 1 dpf with 100 cells/mL of Acinetobacter, Comamonas, or Comamonadaceae resulted in behavioral profiles that were identical to colonized control larvae at 8 dpf. In comparison, axenic embryos colonized with Vibrio bacteria were hypoactive relative to control larvae. Vibrio-related hypoactivity was prevented in axenic larvae colonized with 25 cells/mL each of Actinetobacter, Vibrio, Comamonas, and Comamonadaceae at 1 dpf. Finally, Vibrio-related hypoactivity was found to persist in 10 dpf larvae. These data suggest that specific bacterial taxa are needed to drive normal neurobehavioral development while colonization with other strains may result in behavioral hypoactivity. These findings raise the possibility that environmental chemicals may disrupt neurobehavioral development by selecting for specific classes of host-associated microbes. This abstract does not represent EPA policy.

ORD-023859	Laughlin, S., J. Grossman, A. Marcotte, S. Newton, A. McEachran, A. Williams, E. Ulrich, and J. Sobus. 12 Evaluating the Chemical Space of House Dust, Human Serum, and Silicone Wristband Passive Samplers Using Suspect Screening Analysis. To be presented at 27th Annual Meeting International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Human exposure to synthetic chemicals is a continuing public health concern as many compounds have yet to be fully evaluated for safety. As the number of chemicals continues to increase, environmental health scientists are working to rapidly identify which chemicals are most likely to pose health risks. Current tools supporting rapid risk-based chemical prioritization include high-throughput (HT) exposure monitoring and modeling. The standard analytical tool for HT exposure monitoring is high resolution mass spectrometry. This tool facilitates suspect screening analysis (SSA), a method used to identify large numbers of known chemicals in environmental and biological samples. This presentation describes the use of liquid chromatography mass spectrometry (LC-MS) and state-of-the-art SSA techniques to evaluate chemicals within extracts of standardized human serum, house dust, and silicone wristband passive samplers. Molecular features in these extracts were first identified using full scan MS spectra and then assigned chemical formulae using the US EPA Distributed Structure-Searchable Toxicity (DSSTox) database. Formulae were then batch-searched against known structures using the US EPA CompTox Chemistry Dashboard. Additional data, including exposure and bioactivity information, were available for many of the tentative structures and used to prioritize candidates for MS/MS analyses. All probable structures, based on MS/MS results and other diagnostic criteria, were cross-referenced against chemical standards with existing calibration data. Using structural similarity scores, calibration curves for standards were assigned to probable compounds in the media and used to produce concentration estimates. These screening-level results were ultimately compared to those previously obtained using targeted methods. The methods and results presented here demonstrate SSA as a viable technique for rapid identification and quantification of novel compounds in high-interest media.

ORD-021233	Leonard, J., and C. Tan. Complementing in vitro hazard assessment with exposure and pharmacokinetics considerations for chemical prioritization. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 17.01.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Traditional toxicity testing involves a large investment in resources, often using low-throughput in vivo animal studies for limited numbers of chemicals. An alternative strategy is the emergence of high-

throughput (HT) in vitro assays as a rapid, cost-efficient means to screen thousands of chemicals across hundreds of pathway-based toxicity endpoints and to aid in chemical prioritization for more extensive testing. Such HT in vitro methods, along with integration of HT in silico predictions of population exposure levels and pharmacokinetic (PK) characteristics, act as the foundation for HT risk assessment. Underlying uncertainties in predicted exposure concentrations or PK behaviors could significantly influence the prioritization of chemicals, though the impact of such influences is unclear. In the current study, a framework was developed to incorporate absorbed doses, clearance, and in vitro dose-response data into a PK/pharmacodynamic (PD) model to allow for placement of chemicals into discreet priority bins. In addition, both measured (from literature) and predicted values for absorbed doses or clearance were used in the PK/PD model to evaluate the impact of their uncertainties on the prioritization process. Scenarios using predicted absorbed doses resulted in a larger number of bin misassignments than scenarios using predicted clearance rates, when compared to placement of chemicals into bins using literature-reported values. Prioritization is more robust to uncertainties in clearance due to physiological constraints, whereas the large magnitude of differences between exposure predictions resulting from numerous possible exposure scenarios is the cause of increased errors in prioritization of chemicals into bins.

ORD-023847	Lindstrom, A., M. Strynar, M. Sun, L. McMillan, D. Knappe, and J. Lang. GenX and Other Poly and Perfluoroalkyl Substances (PFAS) in Surface and Drinking Water in North Carolina. To be presented at North Carolina's 19th Annual Community-Based Environmental Justice Summit, Franklinton Center at Bricks, NC, USA, 10/20/2017 - 10/21/2017.	EMMD	Abstract	SSWR 6.01D

Impact / Purpose Statement

Presented at North Carolina's 19th Annual Community-Based Environmental Justice Summit, Franklinton Center at Bricks, NC, USA, 10/20/2017 - 10/21/2017.

Product Description / Abstract

The Cape Fear River system is the source of drinking water for more than 300,000 people in New Hanover, Brunswick, and Pender Counties, but it also receives wastes from urban and rural runoff, municipal wastewater treatment plants, septic systems, and discharges from many industries. These waste inputs are regulated, and finished drinking water is required to meet safety standards that are assumed to be protective of public health, but delivered water can still be contaminated with hazardous pollutants. The discovery of GenX and other related contaminants in finished drinking water supplied to the citizens of southeastern North Carolina illustrates this point precisely. A careful evaluation of this situation highlights some of the key vulnerabilities in our drinking water system, including: siting of large scale industrial operations in rural communities, complex discharge permitting requirements, difficulty of measuring hazardous pollutants in waste streams, environmental persistence of many chemical contaminants, and limited treatment options at drinking water plants. Because these vulnerabilities are well known, many communities have established stringent watershed protections that limit commercial development and industrial discharges in their watersheds. Other communities have little to no control of what their upstream neighbors release into their source water. This presentation summarizes our current understanding of the GenX issue and explores why specific communities may be vulnerable to contamination.

ORD-023607	Liu, X., K. Krebs, M. Allen, K. Thomas, M. Strynar, and D. Greenwell. Characterization of Formaldehyde Emissions from Tire Crumb Rubber in Small Environmental Chambers. Presented at International Society of Exposure Science (ISES) 2017, Research Triangle Park, North Carolina, USA, 10/15/2017 - 10/19/2017.	SED	Poster	SHC 2.62.2

Impact / Purpose Statement

Cleared by NRMRL.
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Concerns have been raised about the safety of recycled rubber tire crumbs used in synthetic turf fields and playgrounds in the United States. To support federal efforts to better characterize recycled tire-derived surface materials, dynamic small chamber tests were conducted at the US EPA National Risk Management Research Laboratory Small Chamber Facility to measure potential formaldehyde emissions from tire crumb rubber materials collected from nine tire recycling facilities and forty synthetic turf fields around the U.S. During tests, approximately 15 grams of tire crumb rubber materials were placed in the center of a 53 L dynamic emission chamber on an aluminum weighing pan for 24 hours before air samples were collected using 2,4-dinitrophenylhydrazine (DNPH) cartridges sampling at a rate of 200-400 mL/min for 90 minutes. The emission chambers were housed in temperature-controlled incubators. An OPTO 22 data acquisition system continuously recorded mass flow controller outputs, temperature, and relative humidity (RH) in the chamber and inlet air. Tests were conducted (N=82) under two chamber conditions, respectively. Formaldehyde concentrations were determined by solvent extraction and analysis by HPLC with Diode-Array Detector. Chamber background and field blank samples were collected for each test. DNPH-formaldehyde detection in selected samples was confirmed by LC/TOFMS. In addition, six duplicates and two time series tests were performed under each set of chamber conditions. The results show that measured formaldehyde concentrations in the chamber at 1 h-1 air change (ACH) rate, 25 °C, 46 % RH, were low and close to the chamber background level. Formaldehyde concentrations measured in the chamber at 1 h-1 ACH, 60 °C, 6.6 % RH, which may represent synthetic field surfaces under hot ambient conditions, were greater than the chamber background for most of the material samples. This research will provide important information for further human exposure study.

ORD-021425	Marcotte, A., S. Laughlin-Toth, J. Grossman, J. Sobus, and E. Ulrich. Suspect Screening and Non-Targeted Analysis of Coupled Soil and House Dust Samples. To be presented at International Society of Exposure Science, Raleigh Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Understanding human exposure to man-made chemicals often requires analyses of indoor environments, where people spend the majority of their time. Coupling indoor and outdoor samples is useful in determining chemicals unique to inside the home, have been transported into the home from outdoor sources (e.g., herbicides), and found only outside which may pose risks to children via dermal contact and indirect ingestion. Here, fifty-six paired outdoor soil and indoor house dust samples, as part of the 2005-2006 American Healthy Homes Survey (AHHS), were analyzed for organic compounds using suspect screening (SSA) and non-targeted analyses (NTA). SSA and NTA are powerful methodologies which use high-resolution mass spectrometry, in this case liquid chromatography quadrupole-time-of-flight mass spectrometry, to identify unknown chemicals in a sample. Molecular features consisting of resolved chromatographic peaks and associated spectra were extracted from raw positive and negative mode data using Agilent Profinder software, revealing several thousand unique features in soil and dust. A subset of these features was matched to chemicals in the Distributed Structure-Searchable Toxicity Database (DSSTox) and assigned tentative identities using the US EPA’s CompTox Chemistry Dashboard. A portion of the unmatched molecular features was prioritized based on normalized abundance and detection frequency and was incorporated into an inclusion list for semi-targeted, data-dependent MS/MS analysis for structural elucidation. For risk assessment purposes, tentatively identified candidates were designated as high-priority based on a ranking scheme including abundance, exposure and toxicity data. Comprehensive SSA and NTA are necessary to fully understand and map the vast network of human exposure. This study identifies the most prevalent compounds found inside and outside the home and those which could be of human health concern due to provisional exposure and bioactivity estimates.

ORD-021327	McEachran, A., J. Grossman, S. Newton, K. Isaacs, K. Phillips, N. Baker, C. Grulke, J. Sobus, and A. Williams. Using the US EPA’s CompTox Chemistry Dashboard to advance non-targeted analysis and exposure research (ISES). Presented at ISES 27th Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01; CSS 18.01.01

Impact / Purpose Statement

Cleared by NCCT

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The use of high resolution mass spectrometry (HRMS) and non-targeted analyses (NTA) is advancing exposure science by enabling researchers to more completely define the exposome. However, confident structure identification of unknowns in NTA continues to present challenges to analytical chemists. Identification requires the integration of complementary data types to generate confident consensus structures; these data include the use of reference databases and source ranking algorithms, fragmentation prediction tools, and retention time prediction. The aim of our research is to generate and implement an identification tool and workflow for NTA within the US EPA’s CompTox Chemistry Dashboard (https://comptox.epa.gov), a chemistry resource and web application containing chemistry data on ~750,000 substances. Data for chemical identification were incorporated from a variety of sources, including: functional use prediction models, PubMed references, and environmental media occurrence models. Data were assembled and a scoring-based identification scheme was empirically developed such that true positives were identified at the top of candidate chemical lists.

This scheme was evaluated using two test sets: a known test set of chemicals and a blinded, unknown mixture. This scoring method for tentative and probable identification of unknowns resulted in increased identification performance over previous workflows. We will discuss development of a visualization tool within the Chemistry Dashboard where users can visualize the relative contributions of identification-specific metrics on a list of candidate structures. The scoring-based method and visualization tools indicate the capability of NTA structure identification within the Dashboard and provide an open, accessible tool for exposure scientists and mass spectrometrists. This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

ORD-023934	Mills, D., A. Marcotte, J. Sobus, K. Hibbert, N. Tulve, and E. Ulrich. Exploring Children’s Chemical and Non-Chemical Stressors by Non-Targeted Analysis of House Dust. To be presented at International Society of Expsoure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	SHC 2.63.1

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Children are at higher risk for adverse health outcomes because of their developing physiology and activities and behaviors, as compared to adults. Additionally, they have increased exposure to chemicals found in house dust due to the amount of time spent indoors, specifically on floors, and child-specific behaviors (e.g., mouthing activities). A pilot study was undertaken to understand whether chemicals found in house dust can indicate exposure to non-chemical stressors (e.g., poor nutrition). A non-targeted analysis method was used to examine dust samples collected from two distinct areas of the same home (upstairs and downstairs locations). Samples were sieved into two particle size fractions (<150 μm and 150 μm-1 mm), extracted in methanol and analyzed using LC/Q-TOF/MS. Over 10,000 unique aligned features were identified and 1,782 total features from both ionization modes (769 negative and 1,013 positive) matched to the U.S. EPA’s DSSTox database and were further investigated using the U.S. EPA’s CompTox Chemistry Dashboard. Spearman correlation coefficients showed near perfect agreement (r=0.98) between features across the two size fractions (26 vs. 55 unique features for small and large), and strong agreement (r=0.86) between features in upstairs vs. downstairs samples (150 vs. 139 unique features). Together, these results indicate high similarity for chemicals adsorbed to dust particles throughout the house. Based on tentative chemical assignments, the chemical stressors in highest abundance are classified as flame retardants, plasticizers, pesticides and personal care products. Further investigations will include the analysis of additional dust samples to focus on: 1) which size fraction and sample location provides more information regarding children’s exposure; 2) whether or not tentatively-identified chemicals can be used as surrogates for non-chemical stressors; and 3) the likely sources of tracer compounds that relate to non-chemical stressors.

ORD-021135	Morgan, M., M. Nash, D.B. Barr, and J. Sobus. Variability of bisphenol-A concentrations in first morning, bedtime, and 24-hour urine samples in 50 North Carolina adults over a six-week period. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	CSS 18.03.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Bisphenol-A (BPA) is a high-production volume chemical that is used to make a number of consumer products and packaged goods. Many cross-sectional studies have frequently reported detecting BPA in urine. However, limited data exist on the temporal variability of urinary BPA concentrations. The major objectives of this study were to: 1) quantify the levels of BPA in first-morning void (FMV), bedtime, and 24-hour samples as concentration, specific gravity (SG) corrected, creatinine (CR) corrected, and excretion rate values for 50 adults over a six-week monitoring period; and 2) determine if these correction approaches decreased the variability in urinary BPA levels. In 2009–2011, a convenience sample of 50 adults (19–50 years old) was recruited from residential settings in North Carolina. Participants collected urine samples (FMV, bedtime, and 24-hour) during weeks 1, 2, and 6 of the six-week monitoring period. Urine samples (n=2335) were analyzed for total BPA concentrations by high-performance liquid chromatography/tandem mass spectrometry. The preliminary data show that BPA was frequently detected (98%) in all of the urine samples. Median levels of BPA were consistently the highest in 24-hour samples (2.08 ng/mL, 2.36 ng/mL-SG, 2.53 ng/mg-CR, and 2.64 ng/min) and the lowest in FMV samples (1.73 ng/mL, 1.61 ng/mL-SG, 1.64 ng/mg-CR, and 1.38 ng/min) across all four methods. Intraclass correlation coefficient (ICC) estimates for BPA showed poor reproducibility (< 0.40) for all urine sample types and methods over a day, week, and six weeks. The highest ICC value of 0.40 occurred for CR-corrected bedtime voids collected over a week. To obtain a reliable average biomarker estimate (ICC=0.80) for BPA, these results indicate that at least six bedtime urine measurements would be needed per adult over a week. In conclusion, these results suggest that bedtime voids may be the preferred sample type to collect in future studies to adequately assess BPA exposures in adults.

ORD-023936	Nelson, C. Relating Soil Geochemical Properties to Arsenic Bioaccessibility Through Hierarchical Modeling. To be presented at International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	SHC 2.62.1

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Arsenic (As) is the highest prioritized contaminant at U.S. Superfund sites. Estimating the site-specific bioavailability of As in soil, defined in this context as the fraction of ingested As that crosses the gastrointestinal epithelium and becomes available for distribution to internal tissues, improves the

accuracy of exposure assessments to evaluate human health risks from As-contaminated soils. Soil geochemical properties influence As bioavailability. Interest in improved understanding of these relationships has motivated the use of regression models to evaluate the ability of soil properties to estimate the amount of As that dissolves from the soil matrix upon exposure to gastric-like conditions, a surrogate measure of bioavailability termed bioaccessibility. However, limits in the numbers and types of soils included in previous studies restrict the usefulness of previous models beyond the range of soil conditions evaluated, as evidenced by reduced predictive performance when models were applied to new data. In response, we developed a novel hierarchical model that can account for variability between contaminant sources and geographic locations to evaluate the ability of soil geochemical properties to estimate As bioaccessibility in 139 soils collected from 97 locations across three continents. This approach improved the estimation of As bioaccessibility in study soils and enabled the identification of a larger suite of elements as significant explanatory variables when compared to previous studies, reflecting the complexity of geochemical mechanisms that control As bioaccessibility across the range of soil properties and contaminant sources encountered in the environment. The hierarchical framework provides a promising approach for improved understanding of the relationships between soil geochemical properties and site specific soil metal bioavailability, with applications for improved risk characterization and remediation of metal(loid)-contaminated soils.

ORD-021492	Newton, S., R. McMahen, J. Sobus, A. Williams, A. McEachran, and M. Strynar. Suspect Screening Analysis of Drinking Water Using Point-of-Use Filters. To be presented at International Society of Exposure Science, Durham, nc, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Despite remarkable progress in recent years in the identification of unknown compounds using high resolution mass spectrometry (HRMS), monitoring programs for drinking water rely on targeted methods which cover a limited number of compounds. In an effort to advance suspect screening analysis (SSA) methodologies and more fully characterize the drinking water exposome, point-of-use water filtration devices (BritaTM filters) were employed to collect time-integrated (1-2 months) drinking water samples in a pilot study of nine central North Carolina homes. Filters were Soxhlet extracted and analyzed by HPLC-TOFMS. Formulas corresponding to observed molecular features (i.e., unknown compounds described by accurate mass, retention time, and mass spectra) were searched against the US EPA’s CompTox Chemistry Dashboard, a recently developed web application and data hub for ~750,000 chemical substances. Out of 14,922 molecular features identified in the samples, 430 were assigned molecular formulas with a match score > 90, which mapped to 10,621 candidate compounds. These compounds were ranked by number of data sources and given a “ToxPi” score calculated using four elements: bioactivity data from EPA’s ToxCast program, exposure estimates from EPA’s ExpoCast program, detection frequency, and average peak area. Of all the candidate compounds, 91 were found as having the highest number of data sources, as well as the highest ToxPi ranking for their molecular formula, and thus grouped as the highest priority compounds. Of these, 15 were confirmed as being correctly identified using standards on hand. Product-use categories from EPA’s CPCat database, again available via the CompTox Dashboard, revealed that the majority of priority compounds are associated with industrial processes

which indicates that drinking water in central North Carolina may be impacted by local industries. Most of the priority compounds would not have been discovered without the use of SSA.

ORD-021489	Phillips, K., A. McEachran, K. Isaacs, J. Sobus, A. Williams, and J. Wambaugh. Assessing Plausibility of Tentative Chemical Identifications from Suspect Screening Analyses via Chemical Function. Presented at 2017 ISES Annual Meeting, Research Triangle Park, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Suspect screening (SSA) and non-targeted analysis (NTA) have become increasingly useful methods for identifying chemicals in indoor environments, which is where many chemical exposures occur. However, the tentative chemical identifications from these analyses must be confirmed. Traditionally, pure chemical standards might be used for confirmation, but this testing is infeasible for the hundreds to thousands of chemicals indicated by these techniques due to both time constraints and availability of standards. Instead, a sometimes laborious process of matching molecular features to a chemical structure may be employed. Here chemical functional use (i.e., the end role of a chemical in a product) is used to filter out unlikely structural matches as part of SSA. In some cases, manufacturers report the functional use of a chemical in its products, but more often than not, chemicals of toxicological interest have little-to-no use information. To fill in these data gaps, quantitative-structure use relationship (QSUR) models have been applied to chemicals with no known use. These models use the structure and physicochemical properties of a chemical to provide a probability for that chemical serving a functional role. As a case study, in a recent SSA of 100 consumer products with 1639 identified chemicals, 1451 of those were not included in data sources listing chemicals associated with consumer products. Such a low number of hits from these data sources is not surprising as many of these sources would not contain information on chemicals used as fragrances, nor of chemicals contained in household articles. However, by examining functional uses, it was found that 696 of the tentatively identified chemicals had at least one reported functional use or had a valid QSUR prediction indicating that these chemicals could serve a functional role in a product and, therefore, should be considered for future confirmation.

ORD-021487	Phillips, K., J. Wambaugh, C. Grulke, K. Dionisio, and K. Isaacs. Identifying Potential Alternatives using Chemical Functional Use. To be presented at International Society of Exposure Science, Research Triangle Park, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The National Research Council noted in its 2014 report A Framework to Guide Selection of Green Alternatives that “focusing on function can provide opportunities for innovation in safer

chemicals and materials.” This presentation highlights efforts to explore such opportunities. Functional use data was collected for more than 14,000 chemicals from multiple public data sources. Harmonized functions were assigned to all chemicals via hierarchical clustering ensuring that a single functional use was assigned to a single chemical regardless of multiple, but similar, names assigned by the different data sources. These harmonized functions were then used to develop quantitative structure-use relationship models which use a chemical’s structure and physicochemical properties to predict whether or not a chemical could serve any of 41 possible functional roles (e.g., surfactant, fragrance). Using these models, the Tox21 chemical library (consisting of ~8500 chemicals) was screened for chemicals that could serve a functional role in a product. Tox21 provides in vitro, high throughput screening data of chemical bioactivity. Tox21 bioactivity was used to compare chemicals with novel predicted uses with chemicals that were already known to be serving that functional role. Chemicals with lesser bioactivity that serve the same role become potential substitutes. These methods have identified more than 1600 candidate alternatives that could undergo higher-tier screening as safer, greener chemical alternatives.

ORD-021447	Price, P. Defining the relationship between individuals’ aggregate and maximum source-specific exposures. Presented at 2017 ISES Annual Meeting, RTP, Noth Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	N/A

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The concepts of aggregate and source-specific exposures play an important role in chemical risk management. The concepts of aggregate and source-specific exposures play an important role in chemical risk management. Aggregate exposure to a chemical refers to combined exposures from all sources and source-specific exposure refers to exposures from a specific source of a chemical. Both types of exposures can occur by multiple routes and exposure pathways and both can be determined on a population and individual level. The issue for aggregate and source-specific exposures is that while an individual’s source-specific exposures may all be acceptable, an individual’s aggregate exposure may not. Examples of regulatory issues that reflect this relationship include the “relative source contribution” used in setting ambient water quality standards, the regulation of sources under the Toxic Substances Control Act within a framework of aggregate exposure, and the assessment of impacts for life-cycle impact assessments. This talk presents a method (Maximum Aggregate Ratio or MAR) for evaluating the relationship between the two metrics. MAR is defined as the ratio of an individual’s aggregate dose to the maximum source-specific dose received by the individual. The MAR can be viewed as a parallel concept to the Maximum Cumulative Ratio (MCR)1,2,3,4 used in mixture risk assessments. The MAR can be used to explore the relationship between interindividual variation in source-specific doses and interindividual variation in aggregate exposures and the impacts of controlling smaller sources on aggregate exposures. A case study of the use of MAR to assess aggregate exposures to chemicals present in different types of consumer products is provided.

ORD-023949	Pye, H., A. Zuend, and G. Isaacman-Van-Wertz. What Aerosol Water do Organic Compounds See?. Presented at AAAR Fall Meeting, Raleigh, North Carolina, USA, 10/18/2017 - 10/18/2017.	CED	Presentation	ACE AIMS-1.5

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

Large amounts of aerosol water are associated with inorganic salts such as ammonium sulfate with generally smaller but important contributions from hydrophilic organics. Ambient aerosols can be externally or internally mixed in addition to containing one or multiple phases. The degree to which organic compounds in a particle interact with water associated with inorganic salts will influence their partitioning between the gas and aerosol phase as well as opportunity to participate in aqueous chemistry. In this work, we examine the potential for liquid-liquid phase separation, or lack thereof, within PM2.5 particles to affect the partitioning of compounds between the gas and aerosol phases. We examine partitioning of ammonia and several isoprene- and monoterpene-derived organic compounds using common (absorptive partitioning, ISORROPIA) and advanced (AIOMFAC) approaches to describing gas-aerosol partitioning for conditions during the Southern Oxidant and Aerosol Study (SOAS). We aim to address the degree to which sophisticated techniques accounting for organic-inorganic interactions, deviations in ideality, and phase separation reproduce observations and the information gained.

ORD-021439	Reyes, J., and P. Price. Trends in Cumulative Exposures of Six Phthalates in the United States from 2005 to 2014. Presented at 2017 ISES Annual Meeting, RTP, North Carolina, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	N/A

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Phthalates are utilized in a wide range of consumer goods and are common contaminants in food. Exposures and resulting dosages of individual phthalates vary over time as a result of changes in their use in consumer products and food contact materials. We calculated the trends in screening estimates of daily dose, Hazard Quotient (HQ), Hazard Index (HI), and Maximum Cumulative Ratio (MCR) for a group of six phthalates using the tolerable daily intakes for the compounds and biomonitoring data collected from 2005 to 2014 under the National Health and Nutrition Examination Survey. HQ is the ratio of an individual’s dose of a chemical and the chemical’s permitted dose. HI is the summation of an individual’s HQs. The MCR is the ratio of the HI to the largest HQ for each individual. There was a 2.2-fold decrease in the mean HI over this period (0.34 to 0.15) and a 7.2-fold decrease in the percentage of participants with an HI greater than 1 (5.7% to 0.8%). Decreases in HI were due to the decreases of diethylhexyl phthalate (DEHP) and dibutyl phthalates (DBP). Diisononyl phthalate (DINP) exposure increased between 2005 and 2014 and the remaining three phthalates

remained approximately constant during this period. The phthalate with the greatest frequency of maximum HQ among individuals with HI values greater than 1 in 2005 was DEHP and in 2014 was DINP. While the individual HI values decreased over time, the values of MCRs increased, indicating that the need to consider cumulative exposures has become more important. These findings suggest that there has been a shift in phthalate exposures in the US population, leading to a decrease in HI values. These secular decreases were most pronounced in the groups experiencing the highest phthalates exposures and occurred due to the declines in HQs for DEHP and DBP out weighing the increases in DINP HQs. The views expressed in this abstract are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.

ORD-021460	Saranjampour, P., W. Setzer, C. Barber, K. Isaacs, P. Egeghy, K. Phillips, and J. Wambaugh. 20171015 - Inferring instream loading rates of organic chemicals in United States watersheds from their downstream concentrations (ISES meeting). To be presented at ISES 2017 Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Abstract	CSS 16.02.01

Impact / Purpose Statement

Cleared by NCCT.

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

High throughput human exposure models have already been developed to allow environmental chemicals to be prioritized for additional testing. The purpose of this study is to evaluate the ability of high throughput ecological exposure models to predict concentrations of chemicals in water samples and quantify the uncertainty in their predictions. We examine three “far-field” (environmental fate and transport) models that can predict the water concentrations for thousands of chemicals as a function of instream loading (i.e., environmental release), physical/chemical properties, and geographic descriptors. To use and evaluate these models, we must first predict the instream loading rate. We investigate developing an instream loading model using inference from the 106 chemicals’ downstream concentrations. We perform a multivariate linear regression analysis for instream loading as a function of various descriptors, such as the predictions from the “down-the-drain” module of the High Throughput Stochastic Human Exposure Dose Simulator (SHEDS-HT) model and data available under the EPA Chemical Data Reporting Rule. We analyze estimated geometric mean water concentrations for 106 extensively sampled chemicals in United States watersheds. We examine means calculated at the national level and for regions and sub-regions that are defined by nested watershed boundaries. By developing a calibrated model for instream loading rates for the 106 chemicals, we can extrapolate the far-field model predictions to other organic chemicals with no water monitoring data, including the majority of the 747,000 chemicals in the EPA CompTox Chemistry Dashboard. This model will facilitate prioritizing those chemicals with higher ecological exposure potential for hazard testing and more targeted exposure assessment.

This abstract does not necessarily reflect U.S. EPA policy.

ORD-021521	Silva, R., S. Prince, F. Cochran, A. Neale, K. Rogers, and T. Buckley. Assessing the Effect of the Natural Environment on Subjective Well-being. Presented at 2017 ISES annual meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/16/2017.	EMMD	Presentation	SHC 3.63.1

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Exposure to the natural environment has a potentially large positive influence on human well-being. Thus, there has been growing interest in understanding the well-being benefits derived from that exposure and establishing causal pathways as they relate to physical health, psychological and social functioning, and subjective well-being. Although natural environments - from pristine natural areas to urban green infrastructure - have an objective impact on human beings related to the provision of life-supporting ecosystem services (e.g., air, water, food, etc.), additional effects are influenced by subjective factors, including individual perceptions and behavior, and social context. The objective of this presentation is to contribute to a better characterization of the size of the salutogenic effects of the natural environment in the US, as well as the mediators and modifiers that influence that association.

ORD-021523	Silva, R., T. Buckley, S. Prince, D. Stout, K. Taylor, L. Alston, and P. Egeghy. Study Design using Video Ethnography to Assess Role of Risk Perception in Use of Consumer Products. Presented at 2017 ISES annual meeting, Research Triangle Park, NC, USA, 10/19/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The nature and extent of human exposure to chemicals found in consumer products is strongly influenced by personal choices and product use. However, little is known about the extent to which risk perception factors into product selection and usage. As part of a feasibility study, we will evaluate video ethnography as a way to improve our understanding of exposures to chemicals from household consumer products and the modifying effect of risk perception. By recording individuals in their home environment and capturing their behaviors, attitudes, and opinions through a series of “in-the-moment” questions and prompts, we hope to better understand both the motivations behind specific behaviors and differences between reported and actual behaviors. Nine women between the ages of 35 and 74 years will be recruited for a 10-day monitoring period. Prior to the monitoring period, the field team will train the participants to facilitate familiarity with a video diary guide and to decrease any potential unease with video recording. Using an iPad and the video diary guide, participants will record a set of videos focused on one regularly used consumer product from each of three general product categories: personal care products, home cleaning products, and consumer-applied pesticides. They will demonstrate technique of use and quantity applied and answer questions designed to probe their knowledge and perceptions of exposure and hazard related to the chemical ingredients of those

products. Video recordings will be analyzed to gain insight into motivations behind specific behaviors, with particular attention to risk perception. Self-administered video recording may reduce field deployment costs while increasing a sense of privacy and a more accurate disclosure of behaviors than questionnaires alone. Field deployment will occur during the Spring and Summer of 2017.

ORD-021507	Sobus, J., A. Williams, A. McEachran, J. Grossman, S. Laughlin-Toth, A. Marcotte, M. Russell, J. McCord, D. Mills, S. Newton, E. Ulrich, M. Strynar, J. Wambaugh, K. Isaacs, K. Phillips, G. Patlewicz, K. Mansouri, A. Richard, and C. Grulke. Using High-throughput Screening Data to Guide Exposome Research. To be presented at International Society of Exposure Science 27th Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Non-targeted analysis (NTA) methods serve as primary data collection tools for human exposome studies. Many NTA workflows utilize high-resolution mass spectrometry (HRMS), and proceed by first identifying thousands of features (i.e., unknown compounds identified by accurate mass, retention time, and mass spectra) in a sample set, and then proposing formulae, and ultimately structures for high-interest features. The process of correctly assigning structures to unknown features is challenging and cumbersome. As such, efforts should be focused on features that are most relevant from a human health perspective. The US EPA CompTox Chemistry Dashboard provides a web interface and public access point for high-quality chemistry, exposure, and bioactivity data. It also serves as a critical component of NTA workflows, and supports investigations into chemicals within consumer products, human biological media, and a variety of environmental media. Our workflow: 1) retrieves structures associated with masses/formulae detected in samples (based on HRMS); 2) identifies “probable” structures using a variety of diagnostic criteria; and 3) prioritizes compounds that are of highest interest for follow-up targeted analysis. Prioritization of high-interest compounds relies heavily on the availability of bioactivity data from high-throughput screening assays, such as those data generated by the Federal Tox21 consortium. In instances where these data are not yet available, QSAR and chemical read-across approaches are considered for candidate prioritization. This presentation will describe methods and tools being used by EPA to rapidly identify, prioritize, and quantify novel compounds in high-interest environmental and biological samples. Data generated from these tools will be used to prioritize parent compounds, metabolites, and chemical mixtures for future bioactivity screening and risk evaluation.

ORD-023866	Sobus, J., E. Ulrich, A. Williams, A. Richard, C. Grulke, A. McEachran, S. Newton, M. Strynar, K. Isaacs, and J. Wambaugh. Setting the Stage for EPA’s Non-Targeted Analysis Collaborative Trial (ENTACT). To be presented at 27th Annual Meeting International Society of Exposure Science, Rsearch Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The last decade has witnessed tremendous innovation in the use of alternative methods for evaluating human health risks posed by man-made chemicals. The Federal Tox21 Consortium and US EPA ToxCast program have collectively screened thousands of chemicals for bioactivity across hundreds of assays. Additionally, EPA’s ExpoCast program has developed methods for predicting exposures to many of these same compounds, allowing for efficient risk-based chemical prioritization. On a parallel research track, efforts continue towards advancing knowledge of the human exposome. Rather than focusing prospectively on chemical safety, these efforts aim to identify primary causes/markers of disease, which may include exogenous and endogenous stressors. Due to differences in approaches, a disconnect exists between top-down exposome research and bottom-up high-throughput screening (HTS) efforts. Non-targeted analysis (NTA) tools can bridge this gap, since they can efficiently generate exposure data for compounds never before monitored, thereby enriching the chemical universe examined in risk evaluations and human health studies. Despite the enormous promise of NTA tools, however, benchmark methods do not yet exist, and limited consideration has been given to how NTA methods can be integrated with traditional targeted workflows in a regulatory context. Noting these challenges, EPA has developed an NTA research framework and collaborative trial to actively engage the exposome and HTS research communities. The research trial makes use of chemical substances from EPA’s ToxCast testing library, and aims to identify the most suitable instrumentation, software, databases, methods, and workflows for performing NTA in support of exposome and HTS research. This presentation will introduce the framework and research trial, and describe steps being taken by EPA to cement NTA methods as indispensable public health research tools.

ORD-023943	Sobus, J., J. Grossman, K. Phillips, S. Newton, A. McEachran, A. Marcotte, A. Williams, and E. Ulrich. Using Structural Similarity to Estimate Concentrations of Known Unknowns in Suspect Screening Analyses. To be presented at International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The author did not submit an abstract

ORD-023979	Solomon, P., S. Kaushik, A. Whitehill, S. Ashok, M. Lunden, B. LaFranchi, and D. Herzl. Exploring the Spatial Representativeness of NAAQS and Near Roadway Sites Using High-Spatial Resolution Air Pollution Maps Produced by A Mobile Mapping Platform. To be presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/19/2017 - 10/19/2017.	EMMD	Presentation	ACE 143

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

In the current study, three Google Street View cars were equipped with the Aclima Environmental Intelligence & trade Platform. The air pollutants of interest, including O3, NO, NO2, CO2, black carbon, and particle number in several size ranges, were measured using a suite of fast time-response reference-grade equipment and combined with a data integration system to enable extensive, routine operation. Supplemental measurements that included temperature (T), relative humidity (RH) were also included. These three instrumented automobiles were driven concurrently in a variety of spatiotemporal patterns in Denver, Colorado over 22 days from mid-July to mid-August 2014, including dense driving around the NAAQS and near-roadway sites. Routes were designed to include interconnected and overlapping driving patterns. This presentation will examine pollution concentrations as observed at the stationary sites compared to those measured by the vehicles within a range of up to 2km from the NAAQS site and within a range ~500m of the near-roadway site.

ORD-023883	Stout, D., L. Alston, F. Chen, P. Egeghy, S. Prince, R. Silva, K. Taylor, R. Walker, and T. Buckley. An Overview of the NIEHS-EPA Pilot Study of Exposure to Chemicals in Consumer Products. To be presented at International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Poster	CSS 16.02.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Research to advance the characterization of environmental and chemical exposures through improved exposure assessments, at both the individual and population levels, is a priority identified in the Strategic Research Action Plans for the U.S. Environmental Protection Agency (EPA) and the National Institutes of Environmental Health Sciences (NIEHS). Research priorities related to exposure assessment include the need to evaluate the utility of existing instruments that classify or quantify exposures, and to develop better tools to improve exposure assessment and understand the nature of combined exposures (e.g., mixtures).

Personal care products (PCPs) and other household/consumer products are of interest because of their

widespread use, the efficiency of their delivery, and existing health concerns over their chemical ingredients. Exposure to these chemical ingredients can result through either direct or indirect contact, depending on the use of the product. Over a lifetime, the average consumer may encounter tens of thousands of chemicals used as ingredients in consumer products, many of which are proprietary; thus, a complete picture of the human exposome is challenging.

Given the large number of co-occurring chemicals in these products, new strategies, tools, and techniques need to be developed and evaluated for their utility in assessing exposure. Innovative tools need to be evaluated for their potential contributions to exposure assessment through rapid, cost-efficient methods which allow the simultaneous measurement of multiple chemical agents and gathering of contextual information to inform exposure reduction. These integrated tools and techniques can then be used to refine measurement and predictive modeling methods that support high throughput chemical analysis and exposure assessment.

The pilot study will assess the feasibility of, and guide and refine procedures for a larger exposure study. The initial motivation for this project stemmed from interest in evaluating the reliability of questionnaires administered in the NIEHS Sister Study as the principal exposure assessment tool. The Sister Study is a large cohort study of 50,000+ women who had at least one sister diagnosed with breast cancer and were themselves breast cancer-free at the time of enrollment. The overall power of the pilot study is to evaluate the effectiveness of the survey, measurement and modeling methods for assessing exposures to chemicals in a number of consumer product categories, including personal care, household cleaning and food packaging products.

ORD-023933	Strynar, M. Per- and Poly-Fluorinated Compounds Analysis: Case Study Cape Fear Drainage Basin. To be presented at EPA meeting hosted by Region 4, Athens, GA, USA, 10/17/2017 - 10/18/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement
Presented at an EPA meeting hosted by Region 4, Athens, GA, USA, 10/17/2017 - 10/18/2017.

Product Description / Abstract
The author did not submit an abstract

ORD-021580	Strynar, M., and J. McCord. Non-Targeted Screening and Identification of Chlorination Products in Reclaimed Water. To be presented at International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

In recent years, total water demand and threats to natural water resources have driven interest in sustainable water practices, such as the reclamation and reuse of wastewater. The reclamation process can produce novel transformation products with limited structural or toxicological data. The application of high-resolution mass spectrometry and non-targeted screening techniques can be used to elucidate these unknown products of water reclamation as a step towards understanding the environmental impacts of reclaimed water usage. In this work, water obtained from wastewater treatment effluent, pre- and post- chlorination at North Carolina wastewater facilities, were examined using non-targeted analysis (NTA) approaches to identify novel products formed during the reclamation process. Concentrated water extracts were analyzed by liquid chromatography (LC) coupled to high resolution mass spectrometry (MS). Molecular features, consisting of accurate mass and chromatographic peaks resolved using MS vendor processing software, in these samples were isolated, and then filtered using a statistical data processing workflow in R. The remaining features were assigned tentative molecular formulae and searched against known compounds in the EPA’s CompTox Chemistry Dashboard (https://comptox.epa.gov/dashboard). Assignments were confirmed using a semi-untargeted data-dependent MS/MS and independent targeted MS/MS characterization was carried out for compounds with no positive matches in the database. The identification of these unknown products is an important first step for future explorations of potential human exposure effects.

ORD-021580	Strynar, M., and J. McCord. Non-Targeted Screening and Identification of Chlorination Products in Reclaimed Water. To be presented at International Society of Exposure Science, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement

Cleared by NHEERL.

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Growing evidence indicates that host-associated microbiota modify the toxicokinetics and/or toxicodynamics of environmental chemicals; however, current risk assessment methods do not consider interactions between microbiota and chemical toxicity. We previously reported that microbial colonization is required for normal neurobehavioral development in zebrafish. We therefore hypothesized that neurobehavioral toxicity may be mediated by altered microbial colonization during development. We explored differences in swimming behavior, microbial community structure, and chemical metabolism in axenic (microbe-free) and conventionally colonized zebrafish larvae that were exposed to the antimicrobial triclosan (0.1-0.3 µM) or vehicle (0.4% DMSO) on 1, 6, 7, 8, and 9 days post fertilization (dpf). At 10 dpf, neurobehavioral function was assessed. Triclosan exposure had no effect on locomotor activity in axenic larvae. In comparison, locomotor hypoactivity was observed in conventionally colonized larvae exposed to 0.3 µM, but not 0.1 µM triclosan. Also on 10 dpf, triclosan exposure triggered concentration-dependent shifts in microbial community structure. To understand the temporal dynamics of triclosan-induced hypoactivity, conventionally colonized larvae were exposed to 0.3 µM triclosan in four scenarios: 1 dpf; 1 and 6 dpf; 1 and 9 dpf; or 1, 6, 7, 8, and 9 dpf. Triclosan exposure only caused hypoactivity at 10 dpf in larvae exposed on 1 and 9 dpf or 1, 6, 7, 8, and 9 dpf. As expected, these two groups contained elevated concentrations of triclosan (ng/larva) at 10 dpf compared to larvae exposed to triclosan on 1 dpf as measured by high resolution mass

spectrometry. Ultimately, this study will serve as a test case to apply non-targeted chemical analyses to reveal unique biotransformation products in axenic and conventionally colonized zebrafish exposed to triclosan during development. In summary, these data suggest that triclosan may exert behavioral effects via dysregulation of microbial colonization during development. This abstract does not necessarily reflect EPA policy.

ORD-020341	Tan, C. Frameworks for organizing exposure and toxicity data - the Aggregate Exposure Pathway (AEP) and the Adverse Outcome Pathway (AOP). Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 17.01.01

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
The Adverse Outcome Pathway (AOP) framework organizes existing knowledge regarding a series of biological events, starting with a molecular initiating event (MIE) and ending at an adverse outcome. The AOP framework provides a biological context to interpret in vitro toxicity data; elaboration of prioritization strategies and the development of tiered testing approaches relying on in silico and in vitro tests. The Aggregate Exposure Pathway (AEP) framework organizes exposure data and predictions from multiple sources, starting with a source and ending at a target site of exposure (TSE). The TSE serves as the bridge between the AEP and the AOP, as it describes the state of a stressor at a target site that corresponds to an MIE. Thus, integration of these two frameworks provides a natural linkage from source to outcome. Disclaimer: This abstract has been cleared by the EPA but solely expresses the view of the authors.

ORD-021403	Tan, C., and A. Paini. Physiologically-based kinetic modelling in risk assessment. Presented at 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 17.01.01

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
The European Union Reference Laboratory for Alternatives to Animal Testing (EURL ECVAM) hosted a two-day workshop with an aim to discuss the role and application of Physiologically Based Kinetic (PBK) models in regulatory decision making. The EURL ECVAM strategy document on Toxicokinetics (TK) outlines PBK models as a central feature for their potential use to integrate data generated by in vitro and in silico methods for absorption, distribution, metabolism, and excretion (ADME) in humans and to predict whole-body biokinetic behaviors. Experts were invited to identify, discuss and recommend challenges in application of PBK models to support regulatory risk assessment. The two primary

challenges were i) constructing models that rely on in vitro and in silico methods for parameterization; (ii) assessing model credibility when in vivo kinetic data are not available for model evaluation how to validated or calibrated models with non-animal data. To address these challenges, the experts recommended a best practices workflow for guidance on the use of in vitro and in silico data in PBK models designed to support regulatory decision making. The outcomes of the workshop and recommendations of the experts will be summarized in this presentation. The presentation will also show results from an international survey on application of PBK models in science and regulatory submission. Analysis of the survey data will provide insights into key concerns in the PBK modeling community, so that recommendations can be made to promote the development and acceptance of PBK models in the safety assessment of chemicals.

ORD-021300	Thomas, K., and A. Ragin-Wilson. Panel Discussion: Improving our understanding of exposures at synthetic turf fields and playgrounds using recycled tire materials. To be presented at ISES, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.62.2

Impact / Purpose Statement

Panel Discussion at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

In recent years, there has been growing concern from the public over the use of recycled tire crumb rubber in synthetic turf fields. In response to these concerns, ATSDR, CPSC, and USEPA developed and implemented a Federal Research Action Plan on Recycled Tire Crumb Used on Playing Fields and Playgrounds (FRAP). The research conducted under the FRAP is intended to provide information about the composition of tire crumb rubber, human exposure activities for field and playground users, and exposure characterization and personal exposure measurements, including personal air monitoring and dermal wipe sampling, among high-end field users. Moreover, previous and ongoing research in the U.S. and Europe provide additional insights for human exposure assessment.

The panel will bring together researchers from the US and Europe, and the discussion will provide an opportunity to explore strengths and weaknesses of existing information, future research directions, and the adequacy of exposure data for risk evaluations. Insights on challenges associated with conducting research on the topic area will be discussed. Panel members will also briefly discuss ongoing research activities, including community outreach and engagement efforts and areas for potential collaboration across agencies.

ORD-021239	Thomas, K., E. Irvin-Barnwell, A. Guiseppi-Elie, and A. Ragin-Wilson. Characterizing Tire Crumb Rubber for Exposure Assessment. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.62.2

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Tire crumb rubber derived from recycled tires is widely used as infill material in synthetic turf fields in the United States. An estimated 95% of the over 12,000 installed fields in the U.S. use tire crumb rubber infill alone or mixed with sand or alternative materials. Concerns have been raised about exposures of field users to the many potential tire chemical constituents. Most previous U.S. research studies examining tire crumb rubber at synthetic fields have been relatively small, restricted to a few fields or material sources, and limited chemical constituents measured. Characterizing chemical, physical, and microbiological constituents and properties for tire crumb rubber is needed to improve human exposure assessment. Working under the U.S. Federal Research Action Plan, researchers collected tire crumb samples from nine tire recycling plants and 25 outdoor and 15 indoor synthetic turf fields across the U.S. Field ages ranged from new installations to 12 years old. Tire crumb samples were analyzed for metals using acid digestion and ICP/MS. SVOCs were extracted with 1:1 hexane/acetone followed by GC/MS and LC/MS analyses. Dynamic chamber tests measured VOC and SVOC emissions at 25° and 60°C. SVOC and VOC analyses included both targeted analyses for chemicals of interest (e.g. polyaromatic hydrocarbons) as well as non-targeted analyses to more fully characterize chemical constituents. Particle size, moisture content, and sand fraction were characterized. Bioaccessibility tests were performed for metals and SVOCs using simulated saliva, sweat, and gastric fluids. Tire crumb rubber samples were found to contain many metal, SVOC, and VOC chemicals across a wide range of concentrations. Chemical constituent information is important but not sufficient for assessing human exposures. Material variability, environmental conditions, bioaccessibility, and human activity factors are among the complex parameters needed to understand exposures at synthetic turf fields.

ORD-021316	Tulve, N., K. Hibbert, and J. Ruiz. Importance of Considering Non-Chemical Stressors in Interpreting Pesticide Exposures in Children. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.1

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Children are exposed to chemical and non-chemical stressors from their total environment, which is comprised of the built, natural, and social environments from places where they spend their time, including home, school, and daycare. Evidence in the literature suggests that the interrelationships between chemical and non-chemical stressors impact their health and well-being in ways that are different from exposure to a single stressor. Our objective was to explore the pesticide literature and evaluate the importance of non-chemical stressors in interpreting young children’s exposures to pesticides and neurocognitive health. We identified publications containing pesticide data, information on non-chemical stressors, and children’s neurocognitive health. We mined the literature, extracted relevant information, created a database, and conducted statistical analyses. We organized the information into stressors from the built, natural, and social environments. Various pesticides (e.g., mirex, chlorpyrifos, DDT) or pesticide metabolites (e.g., dialkyl phosphates) have been studied to

understand the relationship between exposure and children’s neurocognitive health. Our preliminary results showed inconsistent associations between pesticide exposure and children’s neurocognitive health, suggesting that chemical exposures alone may not always be able to explain observed health effects. The complexities of multiple stressors suggest that the interrelationships between chemical and non-chemical stressors should be incorporated into studying children’s neurocognitive health.

ORD-021287	Tulve, N., M. Clifton, S. Vesper, P. Egeghy, K. Thomas, E. Ulrich, D. Stout, K. Isaacs, D. Werthmann, and F. Rabito. Young Children’s Exposures to Molds and Consumer Product Ingredients in their Homes. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.1

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Young children’s physiology and unique interactions with the environment have been shown to influence their exposures to common chemical and biological agents. Many types of consumer products are present in homes, resulting in the potential for direct and indirect exposures to multiple agents. Biological agents present in homes can combine with chemical agents to potentially impact health. Our objective was to examine how lifestage, product use, and building factors affect children’s exposures to selected chemical and biological agents in their home. Multimedia samples (air, dust, surface and hand wipe, sock) and supporting information were collected from 12 children (4-11 years old) living in 8 low-income homes in New Orleans, LA (2016). Surface wipe samples (wipe area=929 cm2) were collected from counters and floors in kitchens and bathrooms. Preliminary consumer product chemical concentrations (pg/cm2) included linalool: 1-8,500; limonene: <MDL-1,250; methyl paraben: <MDL-20,000; propyl paraben: <MDL-13,000; butyl paraben: <MDL-290; triclosan: <MDL-2,000; piperonyl butoxide: <MDL-18,000; permethrin: 1-36,000; fipronil: <MDL-340. Settled dust samples were collected from door jambs and analyzed for mold contamination using a DNA-based analysis. The ERMI (Environmental Relative Moldiness Index) scale, used to measure water damage and predict potential for unhealthy mold conditions, was calculated. The average ERMI value was 5.8 (scale: -10 to 20); however, in 2 homes the ERMI values exceeded 14, indicating mold contamination and potential water damage. All surface wipe samples contained measureable concentrations of the selected chemical agents. These homes showed evidence of water damage and mold growth, with 4 homes in the highest quartile for mold contamination. These preliminary results provide additional evidence that the young children in this pilot study were exposed to a combination of multiple consumer product chemicals and biological agents in their homes.

ORD-021511	Ulrich, E., J. Sobus, A. Richard, C. Grulke, A. Williams, and S. Newton. EPA’s Non-Targeted Analysis Collaborative Research Trial (ENTACT): Evaluating the state-of-the-science for non-targeted analysis. To be presented at International Society of Exposure Science,	EMMD	Presentation	CSS 16.01.01

	Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.			

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
While thousands of chemicals have been profiled for bioactivity using high throughput screening, many of these chemicals are lacking exposure data, which hinders risk-based evaluation. Suspect screening (SSA) and non-targeted analysis (NTA) methods using high-resolution mass spectrometry (HRMS) offer new approaches to efficiently generate exposure data for a growing number of chemicals in commerce in a variety of environmental and biological media. We are conducting EPA’s Non-Targeted Analysis Collaborative Research Trial (ENTACT) to evaluate a range of state-of-the-science SSA and NTA approaches. Four categories of experiments are underway: 1) ten standard chemical mixtures from the EPA’s ToxCast library, 2) extracts of standardized environmental matrices including house dust, human serum, and environmentally deployed silicone passive samplers, 3) extracts of standardized environmental matrices spiked with known chemical mixtures, and 4) approximately 4600 single chemicals from the ToxCast library to produce reference spectra. This presentation will describe the preparation of mixtures, standardized matrices, and single chemical multi-well plates. Approximately 25 laboratories worldwide from academia, government, and private (i.e., vendor) organizations are enrolled in ENTACT. Each laboratory will use their gas and/or liquid chromatography systems and methods to maximize chemical space coverage, provide variations for comparison, and produce both instrument specific and publically available spectral resources. Initial overview results from participating laboratories will be discussed including: methods, software, and databases used; correctly identified chemicals, false negatives, and false positives. The goal of this work is to produce benchmark methods for analytical, reporting, and data analysis to facilitate further analyses and identify areas for improvement.

ORD-021516	Utile, S., N. Tulve, and K. Thomas. A Literature Review and Data Mining Project to Identify Associations between Stressors and Health Outcomes for Children. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.1

Impact / Purpose Statement
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
Children are often more vulnerable than adults to the effects of environmental contaminants found in their everyday environments. Their dynamic growth and unique interactions with the built, natural, and social environments may result in a greater susceptibility to chemical and non-chemical stressors and potential adverse health consequences. Our objective was to examine approaches for evaluating

interrelationships between chemical and non-chemical stressors and children’s health outcomes. Using several search engines (e.g., Google Scholar, Web of Science) and websites (e.g., EPA and NIEHS websites), we compiled over 2400 peer reviewed articles published by the EPA/NIEHS Children’s Environmental Health and Disease Prevention Research Centers (Children’s Centers) for the period 1998-2016. We focused on Children’s Centers publications because of the emphasis on chemical exposures, non-chemical stressors, and multiple child-specific lifestages. Full citations, keywords, and abstracts were entered into an EndNote database. Topic-specific libraries were created for specific chemical (e.g., metals, phthalates, pesticides) and non-chemical (e.g., built environment, food access, cultural practices) stressors and associated health outcomes (e.g., obesity, asthma). Prior to data extraction, manuscripts were reviewed to determine if they contained extractable data, information on chemical and/or non-chemical stressors and the health outcome of interest, and did not pertain to animal studies. Extracted data were entered into a database modeled after the Comparative Toxicogenomics Database. One topic-specific library focused on stressors and childhood obesity, with 156 Children’s Center publications. Of these publications, 14 described chemical (e.g., phthalates, pesticides) stressors and 11 identified non-chemical (e.g., food types) stressors associated with childhood obesity. Preliminary analyses of the childhood obesity and stressors topic specific library will be presented.

ORD-023834	Varghese, A., T. Hong, L. Jessica, H. Hubbard, K. Dionisio, N. Brandon, and P. Price. Product Use Scheduler: A Scheduling Module used in EPA’s Human Exposure Model. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 18.03.01

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

The scheduling model (SM) was developed for scheduling the use of consumer products in the U.S. EPA’s Human Exposure Model (HEM), an integrated modeling system to estimate human exposure to chemicals in household consumer products. The SM begins with year-long daily activity patterns which are produced by a separate module in HEM. These patterns specify the start times and durations for five macro behaviors: sleep, eat, work/school, commute, and idle time (time not spent in the other activities). The SM schedules the use of more than 300 types of products during idle times. The SM determines which of the product types are used in a household based on the characteristics of the household (e.g., house size and type), the characteristics of individuals living in the house (e.g., gender, age, and work status), and the prevalence of product use. The predictions of product use on a given day are then determined for each product type based on seasonality of product use and estimates of frequency and duration taken from the SHEDS-High throughput model. The SM considers whether products are used to satisfy personal or communal needs (frequency is based on the person or household, respectively) and whether a period of idle time is sufficiently long to allow the use of product, and also clusters products typically used at the same time (e.g., toothpaste and mouthwash, paint primer and paint, car wash and car wax). The SM output is a set of activity patterns that specifies the products used on each day of a year by each individual in a household, the durations of product use, and the mass of product used. These estimates are temporally consistent (individuals do not do two things at once), are consistent with longitudinal predictions of macro behaviors, reflect demographic

information, and are consistent with the day of the week and season of the year. The results are used to model human exposure to chemicals in products and the releases of the chemicals to the environment.

ORD-021496	Varughese, E., S. Hunter, D. Shaw, and J. Garland. Addressing Toxicity of Water using the Challenge Process. Presented at 2017 ISES Annual Meeting, Durham, North Carolina, USA, 10/15/2017 - 10/19/2017.	EMMD	Poster	SSWR 6.03B

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Exposure concerns from an increasing number of pollutants in US waters requires the need for better monitoring. The pollutants are diverse and can include pesticides, heavy metals, personal care products, natural toxins such as cyanobacterial toxins, and a host of other organic and inorganic chemical pollutants and their transformation products. Current methods for detecting and identifying many of these contaminants are expensive, time-consuming, and require the use of specialized laboratories. Moreover, multiple methods are needed to detect the variety of contaminants of interest and, if the identity of the potential contaminants is unknown, water monitoring becomes even more complex. A chemically “agnostic” approach to water quality testing could allow for detection of multiple contaminants that are biologically active and trigger specific toxicity or adverse health outcome pathways. Biosensors, (i.e. those sensors which take advantage of biological phenomenon that are altered in the presence of contaminants), can potentially provide faster detection as well as portability, continuous monitoring, and/or detection in complex matrices using minimal sample preparation. The EPA has over the past years used a challenge approach that uses crowd-sourcing to find solutions to difficult problems. The Water Toxicity Biosensor Challenge is a recent task with the goal of producing design solutions for a biologically-based effects monitor/biosensor capable of responding to multiple environmental contaminant exposures that result in toxicity or adverse health effects when host organisms are exposed. This presentation will describe the process as well as provide information related to the challenge of designing a Water Biosensor to analyze the toxicity of water.

ORD-023904	Wambaugh, J., B. Wetmore, K. Mansouri, B. Ingle, R. Tornero-Velez, R. Judson, K. Isaacs, K. Phillips, C. Nicolas, W. Setzer, and R. Thomas. Integrating Toxicity, Toxicokinetic, and Exposure Data for Risk-based Chemical Alternatives Assessment (ISES). To be presented at International Society of Exposure Science annual meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Cleared by NCCT

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

In order to predict the margin between the dose needed for adverse chemical effects and actual human exposure rates, data on hazard, exposure, and toxicokinetics are needed. In vitro methods, biomonitoring, and mathematical modeling have provided initial estimates for many extant chemicals. Providing predictions for novel compounds, however, will need to rely on screening massive chemical libraries and drawing inference from chemical structure (e.g., quantitative structure activity relationships). This presentation will review the challenges and opportunities for alternatives assessment based upon high throughput tools for exposure and hazard. In vitro high throughput screening (HTS) assays, such as the U.S. Federal Tox21 consortium and the U.S. EPA Toxicity Forecaster (ToxCast) program, have generated bioactivity data for thousands of chemicals. For some endpoints (e.g., estrogen receptor and androgen receptor), models trained on these HTS data allow predictions for novel compounds. In tandem with ToxCast, the Exposure Forecaster (ExpoCast) program provides toxicokinetic (TK) data and exposure estimates to provide context for HTS data. Libraries of TK data, largely obtained from in vitro assays, have served as training sets for machine learning models capable of estimating TK for novel compounds. Biomonitoring data obtained by the US CDC National Health and Nutrition Examination Survey and consumer product formulation data have similarly been used to develop models for exposure prediction (mg/kg/day). Integration of these methods provides a timely, risk-based prioritization strategy that characterizes the dose relationships between in vitro bioactivities and predicted human exposure.

ORD-021490	Wambaugh, J., C. Ring, K. Isaacs, K. Phillips, P. Egeghy, and W. Setzer. Predicting Exposure Pathways with Machine Learning (ISES). To be presented at International Society of Exposure Science annual meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/18/2017.	CED	Abstract	CSS 16.02.01

Impact / Purpose Statement

Cleared by NCCT

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Prioritizing the risk posed to human health from the thousands of chemicals in the environment requires tools that can estimate exposure rates from limited information. High throughput models exist to make predictions of exposure via specific, important pathways such as residential product use, diet, and environmental fate and transport. These models can be parameterized in terms of physico-chemical properties that can be predicted with reasonable accuracy from chemical structure. However, as identified by Shin et al. (2015), there are extremely limited data available for identifying the relevant pathways for chemicals in a high throughput manner. Both expert opinion or conservative assumptions (i.e., all chemicals exposed by all pathways) have been considered but have obvious drawbacks. Here we examine the use of machine learning techniques to use structural features and physico-chemical properties to assess the probability that a chemical might be associated with exposure via different pathways. Estimating the relevant pathways using these techniques allows information (including model predictions and other exposure estimates) to be synthesized on a per pathway basis. For each pathway we evaluated the predictive ability of various sources of exposure information using inferred population exposure rates for only those chemicals relevant to the pathway. We can now synthesize exposure models and other predictions commensurate with the ability of those predictions to explain biomonitoring data. In addition, we can attribute the presence of a chemical to specific exposure pathways, potentially allowing structure-based forensic investigation of chemical exposure, and

subsequent remediation.

ORD-023906	Wambaugh, J., J. Sobus, A. Williams, X. Liu, M. Strynar, C. Grulke, A. Richard, E. Ulrich, S. Newton, K. Phillips, K. Isaacs, C. Sonich-Mullin, J. Orme-Zavaleta, R. Thomas, C. Bevington, and C. Fehrenbacher. Generating Exposure-Relevant Measurement Data for Potential Use in Support of TSCA Requirements (ISES). To be presented at International Society of Exposure Science annual meeting, Morrisville, NC, USA, 10/15/2017 - 10/19/2017.	EMMD	Presentation	CSS 16.02.01

Impact / Purpose Statement
Cleared by NCCT
Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
We would like to know more about the potential risk posed by thousands of chemicals in the environment – which ones should we start with? Expanded monitoring data allows model parametrization and evaluation. Are chemicals missing that we predicted would be there? Are there unexpected chemicals? While the amended TSCA provides an opportunity for ORD exposure measurements and databases to support OPPT risk evaluations, prior to any implementation the fitness-for purpose of these projects (e.g., for prioritization, scoping, or risk evaluation) must be evaluated in the context of TSCA requirements.All data being made public.

ORD-021601	Wetmore, B. Opportunities and Challenges in Employing In Vitro-In Vivo Extrapolation (IVIVE) to the Tox21 Dataset. Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement
Course at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract
In vitro-in vivo extrapolation (IVIVE), or the process of using in vitro data to predict in vivo phenomena, provides key opportunities to bridge the disconnect between high-throughput screening data and real-world human exposures and potential health effects. Strategies utilizing a combination of experimental and computational tools to predict chemical and drug toxicokinetics (TK) have shown made significant progress, as have evaluations of the uncertainty and variability of these predictions. A limited understanding of the linkage between in vitro assay bioactivity potencies, target site concentrations and potential downstream apical outcomes contribute to the lack of certainty in the assessment of in vitro toxicodynamics (TD), whether for chemicals or drugs. Data from the Tox21 program, designed to interrogate a discrete set of stress response pathways but across a large swath of chemical space, can be mined to explore the predictivity of IVIVE in assessing the TK and TD across pharmaceutics and

commercial chemicals. This talk will describe recent IVIVE efforts on this dataset, outlining both the opportunities and challenges that have been identified. This abstract does not necessarily reflect U.S. EPA policy.

ORD-021604	Wetmore, B., A. Williams, R. Judson, and J. Wambaugh. Using US EPA’s Chemical Safety for Sustainability’s Comptox Chemistry Dashboard and Tools for Bioactivity, Chemical and Toxicokinetic Modeling Analyses (Course at 2017 ISES Annual Meeting). Presented at 2017 ISES Annual Meeting, Durham, NC, USA, 10/15/2017 - 10/19/2017.	CED	Presentation	CSS 16.02.01

Impact / Purpose Statement

Course at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Course Abstract: Ongoing research within the US EPA’s Chemical Safety for Sustainability program strives to integrate advances in in vitro experimentation, biotechnology, and in silico tools and modeling to evaluate chemicals for potential human health issues. Efforts have included compilation of information across multiple data streams for thousands of chemicals to capture physical-chemical properties, high-throughput bioactivity data, pharmacokinetic properties, consumer use, product and exposure information along with predictive computational tools developed to predict potential hazard and exposure. These data and tools are publicly available through the EPA’s web-based CompTox Chemistry Dashboard, which also provides links to many other EPA databases, tools and public websites. This course will introduce students to these resources and provide guidance on how they can be mined to aid in chemical and biological data mining, pharmacokinetic modeling, and in vitro-in vivo extrapolation efforts to link assessments of in vitro exposure and toxicity to in vivo exposures.

ORD-021271	Zartarian, V., J. Xue, R. Tornero-Velez, J. Brown, T. Speth, and J. Garland. Childhood Multimedia Lead Exposures: Innovative Modeling and Data Collection Efforts by the Federal Family to Guide Public Health Decision-Making. To be presented at ISES 2017 Annual Meeting, Research Triangle Park, NC, USA, 10/15/2017 - 10/19/2017.	SED	Presentation	SHC 2.63.6

Impact / Purpose Statement

Presented at the 2017 ISES Annual Meeting, Research Triangle Park, NC, USA, 10/16/2017 - 10/19/2017.

Product Description / Abstract

Drinking water and other sources for lead are the subject of public health concern following the Flint, Michigan drinking water and East Chicago, Indiana lead in soil crises. In 2015, the U.S. EPA’s National Drinking Water Advisory Council recommended establishing a “health-based, household action level” for children based on exposure to lead in drinking water. A modeling approach, coupling the EPA’s SHEDS-Multimedia and IEUBK models was developed to help determine what

drinking water lead concentrations keep children’s blood lead levels (BLLs) below specified values, considering exposures from water, soil, dust, food, and air. Related objectives were to evaluate the model estimates using real-world blood lead data; quantify relative contributions by the various media; and identify key model inputs. This analysis for the U.S. population of young children probabilistically simulated multimedia exposures and estimated relative contributions of media to BLLs across all population percentiles for several age groups. Modeled BLLs compared well with nationally representative BLLs (0%-23% relative error). Analyses revealed the relative importance of soil and dust ingestion exposure pathways, and associated lead intake rates; water ingestion was also a main pathway, especially for infants. Given the spatial and temporal variability of household lead water concentrations, there are uncertainties in water lead concentration data collected under the current regulatory sampling schemes. Local-scale data for the various multimedia model inputs and BLLs would be beneficial for extending the coupled model approach to other applications and specific communities. This methodology advances scientific understanding of the relationship between lead concentrations in drinking water and BLLs in children.

ORD-021362	Zhang, Y., J. West, R. Mathur, J. Xing, C. Hogrefe, S. Roselle, J. Bash, J. Pleim, M. Gan, and D. Wong. Significantly reduced health burden from ambient air pollution in the U.S. under emission reductions from 1990 to 2010. To be presented at 36th AAAR conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.	CED	Presentation	ACE AIMS-1.4

Impact / Purpose Statement

Presented at the 36th AAAR Annual Conference, Raleigh, NC, USA, 10/16/2017 - 10/20/2017.

Product Description / Abstract

The recent 2013 Global Burden of Disease Study 2013 has attributed the ambient PM2.5 as the fifth-ranking mortality risk factor in 2015. While assessing the global or national burden of disease attributed to air pollution has become more common, fewer studies have tried to understand how these burdens change through time. Here, we aim to use long-term modeling results to quantify how air pollution-related mortality has changed in the U.S. in each year from 1990 to 2010, and to quantify the importance of changes in contributing factors to the long-term trends. We use 21-year historical estimates of PM2.5 and ozone concentrations from 1990 to 2010 simulated with the coupled WRF-CMAQ model with consistent U.S. emission inventories, and annual county-level baseline mortality rates and population archived by the U.S. Centers for Disease Control.

We find that the PM2.5-related health burdens have steadily decreased. The health burden has decreased by 54% from 1990 to 2010. The PM2.5 -related health burdens would decrease only by 26% if the PM2.5 concentrations had not decreased from 1990. The health burden decreases are caused by the combined effect of decrease in baseline mortality rates of major disease and annual PM2.5 concentrations. The health burden associated with O3 has larger inter-annual variations compared with PM2.5-related health burdens, which are dominated by the inter-annual O3 changes. The O3-related health burdens have increased by 28% for the past 2 decades, which is mainly caused by the increases of the baseline mortality rates and the population, despite ozone decreases. The O3-related health burden would have increased by 59% if the O3 concentration was kept constant at the 1990 level.